A Bibliography of ICCMSE 2007

Nelson H. F. Beebe
University of Utah
Department of Mathematics, 110 LCB
155 S 1400 E RM 233
Salt Lake City, UT 84112-0090
USA

Tel: +1 801 581 5254
FAX: +1 801 581 4148

E-mail: beebe@math.utah.edu, beebe@acm.org,
beebe@computer.org
WWW URL: http://www.math.utah.edu/~beebe/

22 March 2018
Version 1.04

Title word cross-reference

References

Ohrn:2007:TDM

[1] Yngve Öhrn. Time-dependent molecular reaction dynamics. In Maroulis and Simos [412], pages 1–9. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000001000001&idtype=cvips`.

Bera:2007:EEE

[2] Partha P. Bera and Henry F. Schaefer III. Elementary energetic effects of radiation damage to DNA and RNA subunits. In Maroulis and Simos [412], pages 10–16. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000010000001&idtype=cvips`.

Economou:2007:LHM

[3] E. N. Economou. Left handed metamaterials: A new frontier in optics? In Maroulis and Simos [412], pages 17–22. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000017000001&idtype=cvips`.

Murakami:2007:CEP

[4] Kazuaki J. Murakami, Feng Long Gu, Mutsumi Aoyagi, Takeshi Nanri, and Koji Inoue. At the cutting edge of a petascale computing world: An overview of petascale system interconnect project. In Maroulis and Simos [412], pages 23–38. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000023000001&idtype=cvips`.

Averbukh:2007:IID

[5] V. Averbukh and L. S. Cederbaum. Interatomic (intermolecular) decay processes in clusters: Current status and outlook. In Maroulis and Simos [412], pages 39–46. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000039000001&idtype=cvips`.

Fowler:2007:MCA

[6] P. W. Fowler. Molecular currents and aromaticity. In Maroulis and Simos [412], pages 47–53. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000047000001&idtype=cvips`.

Wang:2007:EMS

[7] Feng Wang. Electron momentum spectroscopy and its applications to molecules of biological interest. In Maroulis and Simos [412], pages 54–81. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000054000001&idtype=cvips`.

Dejardin:2007:NAD

[8] Jean-Louis Déjardin. Nonlinear ac dielectric response in polyelectrolytes. In Maroulis and Simos [412], pages 82–92. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000082000001&idtype=cvips`.

Lucas:2007:PFP

[9] K. Lucas. Prediction of fluid phase behavior from molecular models. In Maroulis and Simos [412], pages 93–103. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000093000001&idtype=cvips`.

Zhu:2007:MNT

[10] Rui Zhu and Dennis R. Salahub. Mechanisms of nucleotidyl transfer catalyzed by the yeast RNA polymerase II. In Maroulis and Simos [412], pages 104–110. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000104000001&idtype=cvips`.

Datta:2007:ANS

[11] Dipayan Datta and Debashis Mukherjee. Applications of a novel spin-free combinatoric open-shell coupled cluster (COS–CC) theory to single-reference doublets. In Maroulis and Simos [412], pages 111–119. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000111000001&idtype=cvips`.

Aoki:2007:EMA

[12] Y. Aoki, F. L. Gu, Y. Orimoto, S. Suhai, and A. Imamura. Elongation method applied to aperiodic systems-random polypeptides, high spin alignment, polymer in solvent, and DNA. In Maroulis and Simos [412], pages 120–137. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000120000001&idtype=cvips`.

Autschbach:2007:MRP

[13] Jochen Autschbach. Molecular response properties calculated and analyzed using static and time-dependent DFT. In Maroulis and Simos [412], pages 138–167. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000138000001&idtype=cvips`.

Davies:2007:GAS

[14] Teresa E. B. Davies, Mihail M. Popa, and Cristian V. Ciobanu. Genetic algorithm for structural optimization of tubular nanostructures. In Maroulis and Simos [412], pages 168–175. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000168000001&idtype=cvips`.

Norman:2007:ART

[15] Patrick Norman. Applications of response theory with relaxation. In Maroulis and Simos [412], pages 176–206. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000176000001&idtype=cvips`.

Calaminici:2007:TDP

[16] Patrizia Calaminici, Andreas M. Köster, and Gabriel U. Gamboa Martinez. Temperature dependence of the polarizability of sodium clusters: An all-electron density functional study. In Maroulis and Simos [412], pages 207–211. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000207000001&idtype=cvips`.

Scivetti:2007:NQE

[17] Iván Scivetti, David Hughes, Nikitas Gidopoulos, Alfredo Caro, and Jorge Kohanoff. Nuclear quantum effects on the structural properties of solids. In Maroulis and Simos [412], pages 212–223. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000212000001&idtype=cvips`.

Ning:2007:CMF

[18] N. Ning, G. Dolgonos, W. Morscheidt, A. Michau, K. Hassouni, and H. Vach. Computational methods for fundamental studies of plasma processes. In Maroulis and Simos [412],

pages 224–249. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000224000001&idtype=cvips.

Bancewicz:2007:IRH

[19] Tadeusz Bancewicz. Induced Rayleigh and hyper-Rayleigh spectra pair hyperpolarizability. In Maroulis and Simos [412], pages 250–256. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000250000001&idtype=cvips.

Koseki:2007:SOC

[20] Shiro Koseki. Spin-orbit coupling effects in di-hydrides of third-row transition elements. In Maroulis and Simos [412], pages 257–267. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000257000001&idtype=cvips.

McDouall:2007:APM

[21] Joseph J. W. McDouall and David Robinson. Approximate procedures in multireference perturbation theory: Successes and limitations. In Maroulis and Simos [412], pages 268–291. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000268000001&idtype=cvips.

Sekino:2007:DAR

[22] Hideo Sekino and Shinji Hamada. A dynamically adaptive refinement in muliresolution multiwavelet basis for dynamical quantum wavefunctions. In Maroulis and Simos [412], pages 292–295. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000292000001&idtype=cvips.

Picaud:2007:MDM

[23] S. Picaud, P. N. M. Hoang, L. B. Partay, G. Hantal, and P. Jedlovszky. Molecular dynamics and Monte Carlo simulations of organic compounds adsorbed on ice surfaces. In Maroulis and Simos [412], pages 296–307. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000296000001&idtype=cvips.

Loos:2007:FBL

[24] Pierre-François Loos and Xavier Assfeld. On the frontier bond location in the QM/MM description of peptides and proteins. In Maroulis and Simos [412], pages 308–315. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000308000001&idtype=cvips.

Papadopoulos:2007:LNL

[25] Manthos G. Papadopoulos and Aggelos Avramopoulos. The linear and non-linear optical properties of some noble gas compounds. In Maroulis and Simos [412], pages 316–328. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000316000001&idtype=cvips.

Carbonniere:2007:VAQ

[26] Philippe Carbonniere, Alain Dargelos, and Claude Pouchan. Vibrational analysis from quantum mechanic molecular dynamics trajectories. In Maroulis and Simos [412], pages 329–336. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000329000001&idtype=cvips.

Manohar:2007:CVR

[27] Prashant Uday Manohar and Sourav Pal. Constrained variational response to Fock-space multi-reference coupled-cluster theory: Formulation for excited-state electronic

structure calculations and some pilot applications. In Maroulis and Simos [412], pages 337–344. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000337000001&idtype=cvips.

Flores:2007:EFC

[28] Patricio Flores, Soledad Gutiérrez-Oliva, Bárbara Herrera, Eduardo Silva, and Alejandro Toro-Labbé. The electronic flux in chemical reactions. insights on the mechanism of the Maillard reaction. In Maroulis and Simos [412], pages 345–349. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000345000001&idtype=cvips.

Castet:2007:MSSa

[29] Frédéric Castet, Benoît Champagne, Masayoshi Nakano, and Hideaki Takahashi. Multiscale simulations for materials and life sciences. In Maroulis and Simos [412], pages 350–378. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000350000001&idtype=cvips.

Rizzo:2007:RPC

[30] Antonio Rizzo. Recent progress in the computation of nonlinear optical properties of chiral systems. In Maroulis and Simos [412], pages 379–388. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000379000001&idtype=cvips.

Ohta:2007:TAL

[31] Koji Ohta and Kenji Kamada. Theoretical approach to large two-photon absorption cross section in extended π-conjugated systems. In Maroulis and Simos [412], pages 389–405. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000389000001&idtype=cvips.

Ramasesha:2007:MMM

[32] S. Ramasesha and Rajamani Raghunathan. Multiscale modeling of molecular magnets. In Maroulis and Simos [412], pages 406–415. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000406000001&idtype=cvips.

Hobza:2007:CSE

[33] Pavel Hobza. Calculations of the stabilization energies of the building blocks of biomacromolecules. In Maroulis and Simos [412], pages 416–424. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000416000001&idtype=cvips.

Yoshioka:2007:ABM

[34] Yasunori Yoshioka. Applications of B3LYP method for enzyme reactions: O_2 reduction by cytochrome c oxidase and ubiquinol oxidation by cytochrome bc_1 complex. In Maroulis and Simos [412], pages 425–436. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000425000001&idtype=cvips.

Sabin:2007:DAS

[35] John R. Sabin, Remigio Cabrera Trujillo, L. T. Chadderton, N. Yngve Öhrn, and Erik Deumens. Directional aspects of swift ion stopping in a protobiological molecule: Formaldehyde. In Maroulis and Simos [412], pages 437–447. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000437000001&idtype=cvips.

Harris:2007:HCW

[36] Frank E. Harris. Highly compact wavefunctions for four-body systems. In Maroulis and Simos [412], pages 448–459. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000448000001&idtype=cvips.

Morales:2007:CSD

[37] Jorge A. Morales. Coherent-states dynamics: A tribute to N. Yngve Öhrn. In Maroulis and Simos [412], pages 460–473. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000460000001&idtype=cvips.

Zdetsis:2007:SDB

[38] Aristides D. Zdetsis. Similarities and differences between silicon and carbon nanostructures: Theoretical predictions. In Maroulis and Simos [412], pages 474–480. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000474000001&idtype=cvips.

Bieniasz:2007:UVC

[39] L. K. Bieniasz. A unifying view of computational electrochemistry. In Maroulis and Simos [412], pages 481–486. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000481000001&idtype=cvips.

Nikolic:2007:RAT

[40] Sonja Nikolic. Recent advances in the theory of Zagreb indices. In Maroulis and Simos [412], pages 487–490. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000487000001&idtype=cvips.

Altoe:2007:CTQ

[41] Piero Altoè, Marco Stenta, Andrea Bottoni, and Marco Garavelli. COBRAMM: A tunable QM/MM approach to complex molecular architectures. modelling the excited and ground state properties of sized molecular systems. In Maroulis and Simos [412], pages 491–505. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000491000001&idtype=cvips.

Zerbetto:2007:TUD

[42] Francesco Zerbetto. Towards understanding different spatial and temporal scales. In Maroulis and Simos [412], pages 506–512. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000506000001&idtype=cvips.

Elstner:2007:SPT

[43] M. Elstner, M. Hoffmann, and M. Wanko. Simulation of proton transfer processes and excited-state properties in proteins with QM/MM methods. In Maroulis and Simos [412], pages 513–519. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000513000001&idtype=cvips.

Zannoni:2007:CSL

[44] Claudio Zannoni. Computer simulation of liquid crystal materials: From generic to specifically decorated molecular models. In Maroulis and Simos [412], pages 520–525. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000520000001&idtype=cvips.

Serrano-Andres:2007:BPC

[45] Luis Serrano-Andrés, Manuela Merchán, Daniel Roca-Sanjuán, Gloria Olaso-González, and Mercedes Rubio. Bioexcimers as precursors of charge transfer and reactivity in photobiology. In Maroulis and Simos [412], pages 526–532. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000526000001&idtype=cvips`.

Paspalakis:2007:CIP

[46] Emmanuel Paspalakis, Constantinos Simserides, and Andreas F. Terzis. Controlled intersubband population dynamics in a semiconductor quantum well. In Maroulis and Simos [412], pages 533–540. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000533000001&idtype=cvips`.

Thanopulos:2007:LID

[47] Ioannis Thanopulos. Laser-induced dynamical chirality and intramolecular energy flow in the CH chromophore. In Maroulis and Simos [412], pages 541–551. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000541000001&idtype=cvips`.

Muller:2007:HEQ

[48] Carsten Müller, Guido R. Mocken, Karen Z. Hatsagortsyan, and Christoph H. Keitel. High-energy quantum dynamics in ultra-intense laser pulses. In Maroulis and Simos [412], pages 552–559. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000552000001&idtype=cvips`.

Nicolaides:2007:IME

[49] Cleanthes A. Nicolaides, Theodoros Mercouris, and Yannis Komninos. Ab initio many-electron calculation of hyperfast time-resolved coherent excitation and decay of polyelectronic atoms. In Maroulis and Simos [412], pages 560–569. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000560000001&idtype=cvips`.

vanderZwan:2007:TIM

[50] Elmar V. van der Zwan and Manfred Lein. Tomographic imaging of molecular orbitals in length and velocity form. In Maroulis and Simos [412], pages 570–575. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000570000001&idtype=cvips`.

Gonzalez:2007:LCW

[51] Leticia González, Tamás Rozgonyi, David Ambrosek, and Guillermo Pérez-Hernández. Laser control of wavepacket photodissociation and photoisomerization dynamics in isolated molecules. In Maroulis and Simos [412], pages 576–585. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000576000001&idtype=cvips`.

Batzias:2007:TSF

[52] Fragiskos Batzias. Two-step fuzzy multicriteria ranking of whole cells immobilization methods for biosensor/biocatalyst selection/synthesis. In Maroulis and Simos [412], pages 586–595. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000586000001&idtype=cvips`.

Nandy:2007:MCD

[53] A. Nandy. Mathematical characterization of DNA sequences — towards new directions. In Maroulis and Simos [412], pages 596–602. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000596000001&idtype=cvips`.

Ruta:2007:RSD

[54] Dymitr Ruta and Bogdan Gabrys. Reducing spatial data complexity for classification models. In Maroulis and Simos [412], pages 603–613. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000603000001&idtype=cvips`.

Persson:2007:ESS

[55] Ingmar Persson. Experimental structural studies of solutes in aqueous solution. In Maroulis and Simos [412], pages 614–620. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000614000001&idtype=cvips`.

Marcos:2007:CMSa

[56] E. Sánchez Marcos, E. C. Beret, J. M. Martínez, R. R. Pappalardo, R. Ayala, and A. Muñoz-Páez. Coupling MD simulations and X-ray absorption spectroscopy to study ions in solution. In Maroulis and Simos [412], pages 621–626. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000621000001&idtype=cvips`.

Caballero-Gil:2007:GBI

[57] P. Caballero-Gil and A. Fúster-Sabater. Graph-based improvement of edit distance attacks. In Maroulis and Simos [412], pages 627–635. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000627000001&idtype=cvips`.

Manias:2007:ESM

[58] E. Manias and Alexei M. Kisselev. Equation-of-state model for temperature-responsive polymers with tunable response onset. In Maroulis and Simos [412], pages 636–651. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000636000001&idtype=cvips`.

Khokhlov:2007:CDCa

[59] Alexei R. Khokhlov, Yury A. Kriksin, Igor Ya. Erukhimovich, and Pavel G. Khalatu. Computer design of copolymers with desired functionalities: Microphase separation in diblock copolymers with amphiphilic block. In Maroulis and Simos [412], pages 652–658. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000652000001&idtype=cvips`.

Li:2007:SBE

[60] Yiming Li, Shao-Ming Yu, Yi-Ting Kuo, and Yih-Lang Li. Simulation-based evolutionary method in antenna design optimization for WLAN and wireless communication applications. In Maroulis and Simos [412], pages 659–670. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000659000001&idtype=cvips`.

Li:2007:EED

[61] Yiming Li, Su-Yun Chiang, and Kuen-Ying Liou. Evolutionary estimation of diffusion models in multi-generation NAND flash memory using genetic algorithm. In Maroulis

and Simos [412], pages 671–676. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000001000671000001&idtype=cvips`.

Maroulis:2007:RBH

[62] George Maroulis, Ajit J. Thakkar, and K. J. Murakami. The Rodney Bartlett Honor Symposium. In Simos and Maroulis [413], pages 3–5. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000003000001&idtype=cvips`.

Bacalis:2007:UFA

[63] Naoum C. Bacalis. Utilizing the fact that among all trial functions orthogonal to an approximate ground state, Φ^0, the closest, Φ^{1+} to the exact first excited state, ψ^1, has lower energy than the exact: $E[\Phi^{1+}] < E[\psi^1]$. In Simos and Maroulis [413], pages 6–9. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000006000001&idtype=cvips`.

Basak:2007:ITB

[64] Subhash C. Basak, Brian D. Gute, Kevin T. Geiss, and Frank A. Witzmann. Information-theoretic biodescriptors for proteomics maps: Applications to rodent hepatotoxicity. In Simos and Maroulis [413], pages 10–13. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000010000001&idtype=cvips`.

Begue:2007:MIS

[65] Didier Bégué and Claude Pouchan. Modeling the IR spectra of acetaldehyde from a new vibrational configuration interaction method. In Simos and Maroulis [413], pages 14–18. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000014000001&idtype=cvips`.

Dhiflaoui:2007:SSK

[66] J. Dhiflaoui, H. Bouzouita, and H. Berriche. Stability and structure of $Na^+ Kr_n$ ($n = 1$–20) clusters. In Simos and Maroulis [413], pages 19–22. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000019000001&idtype=cvips`.

Mabrouk:2007:TSC

[67] N. Mabrouk, H. Berriche, and F. X. Gadea. Theoretical study of the CsLi molecule beyond the Born–Oppenheimer approximation. In Simos and Maroulis [413], pages 23–27. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000023000001&idtype=cvips`.

Bielinska-Waz:2007:SDD

[68] P. Bielińska-Waż, W. Nowak, A. Nandy, and S. C. Basak. Similarity and dissimilarity of DNA/RNA sequences. In Simos and Maroulis [413], pages 28–30. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000028000001&idtype=cvips`.

Daskalakis:2007:PDS

[69] Vangelis Daskalakis, Stavros C. Farantos, and Constantinos Varotsis. Protein dynamics and spectroscopy for ferryl intermediate of cytochrome *c* oxidase: A molecular dynamics approach. In Simos and Maroulis [413], pages 31–34. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000031000001&idtype=cvips`.

Dkhissi:2007:CTS

[70] Ahmed Dkhissi and Claude Pouchan. Comparative theoretical study of poly[3-(4-octylphenyl)thiophenes] and poly[3-(4-octylphenoxy)thiophenes] as promising photovoltaic cells materials. In Simos and Maroulis [413], pages 35–39. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000035000001&idtype=cvips`.

Domingues:2007:SPHa

[71] Guilherme Domingues, Yoshiyuki Morie, Feng Long Gu, Takeshi Nanri, and Kazuaki Murakami. SMMH — A parallel heuristic for combinatorial optimization problems. In Simos and Maroulis [413], pages 40–43. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000040000001&idtype=cvips`.

Glaz:2007:IHR

[72] Waldemar Głaz, Tadeusz Bancewicz, Jean-Luc Godet, and George Maroulis. Induced hyper-Rayleigh spectra. theoretical and numerical analysis of spectral moments. In Simos and Maroulis [413], pages 44–47. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000044000001&idtype=cvips`.

Bartlett:2007:RDM

[73] R. J. Bartlett, G. Fagas, and J. C. Greer. Reduced density matrices in quantum electronic transport. In Simos and Maroulis [413], pages 48–51. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000048000001&idtype=cvips`.

Gu:2007:IPC

[74] Feng Long Gu, Hyacinthe Nzigou M., Guilherme de Melo Baptista Domingues, Takeshi Nanri, and Kazuaki Murakami. Investigating the performance of collective communications on SMP clusters: A case for `mpi_allgather`. In Simos and Maroulis [413], pages 52–56. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000052000001&idtype=cvips`.

Bai:2007:CCN

[75] Haihua Bai, Chun Li, Hasi Agula, Jirimutu, Jun Wang, and Lili Xing. Cp-curve, a novel 3-D graphical representation of proteins. In Simos and Maroulis [413], pages 57–60. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000057000001&idtype=cvips`.

Hohm:2007:TFD

[76] Uwe Hohm. Are there frame-distortion contributions to collision-induced absorption and collision-induced light scattering? In Simos and Maroulis [413], pages 61–63. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000061000001&idtype=cvips`.

Honda:2007:IEF

[77] Hiroaki Honda, Tetsuo Hayashi, Yuichi Inadomi, Koji Inoue, and Kazuaki J. Murakami. Implementation and evaluation of Fock matrix calculation program on the Cell Processor. In Simos and Maroulis [413], pages 64–67. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000064000001&idtype=cvips`.

Karamanis:2007:EDP

[78] Panaghiotis Karamanis and Demetrios Xenides. Electric dipole polarizability of aluminum phosphide clusters $\mathrm{Al}_n\ \mathrm{P}_n$ ($n = 2$–9) and electron delocalization. In Simos and Maroulis [413], pages 68–71. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000068000001&idtype=cvips`.

Kosmas:2007:CSD

[79] Agnie Mylona Kosmas and Demetrios K. Papayannis. Computational studies on dihalogen complexes of N-methyl imidazoline-2-thione and N-methyl imidazolidine-2-thione. In Simos and Maroulis [413], pages 72–75. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000072000001&idtype=cvips`.

Kosmas:2007:HMN

[80] Agnie M. Kosmas and Antonija Lesar. Halogenated methyl nitrates, CX_3ONO_2 (X = F, Cl). A computational study of their properties and capacity to act as sink compounds in the troposphere. In Simos and Maroulis [413], pages 76–79. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000076000001&idtype=cvips`.

Lindgren:2007:FTA

[81] Ingvar Lindgren, Sten Salomonson, and Daniel Hedendahl. Field-theoretical approach to many-body perturbation theory: Combining MBPT and QED. In Simos and Maroulis [413], pages 80–83. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000080000001&idtype=cvips`.

Makowski:2007:IAT

[82] Marcin Makowski. Improvements in algorithms for two electron repulsion integrals evaluation in Gaussian type basis sets. In Simos and Maroulis [413], pages 84–87. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000084000001&idtype=cvips`.

Mestechkin:2007:PMD

[83] M. Mestechkin. Phenomenological and microscopic description of molecular layer and crystal optical polarization. In Simos and Maroulis [413], pages 88–91. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000088000001&idtype=cvips`.

Minicozzi:2007:RMA

[84] V. Minicozzi, S. Morante, G. C. Rossi, and F. Stellato. The rôle of metals in amyloid aggregation: A test case for *ab initio* simulations. In Simos and Maroulis [413], pages 92–97. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000092000001&idtype=cvips`.

Musia:2007:ECS

[85] Monika Musia. EOM–CCSDT study of the low-lying ionization potentials of CO_2, CS_2 and OCS. In Simos and Maroulis [413], pages 98–101. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000098000001&idtype=cvips`.

Nakano:2007:SHD

[86] Masayoshi Nakano, Ryohei Kishi, Akihito Takebe, Masahito Nate, Hideaki Takahashi, Takashi Kubo, Kenji Kamada, Koji Ohta, Benoît Champagne, and Edith

Botek. Second hyperpolarizabilities (γ) of 1,3-dipole systems: Diradical character dependence of γ. In Simos and Maroulis [413], pages 102–105. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000102000001&idtype=cvips.

Nanri:2007:EPP

[87] Takeshi Nanri, Takeshi Soga, Koji Kurihara, Feng Long Gu, Hiroaki Ishihata, and Kazuaki Murakami. Evaluation of the performance of parallel sparse-matrix multiplication and the effect of dynamic load-balancing. In Simos and Maroulis [413], pages 106–109. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000106000001&idtype=cvips.

Saal:2007:VNM

[88] Amar Saal, Mahfoud Hadj Ben Ali, and Ourida Ouamerali. Vibrational normal modes contributions to the vibrational first hyperpolarizability in a sample of TICT molecules. In Simos and Maroulis [413], pages 110–113. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000110000001&idtype=cvips.

Perera:2007:PQC

[89] Ajith Perera. Predictive quantum chemistry: A step toward "chemistry without test tubes". In Simos and Maroulis [413], pages 114–117. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000114000001&idtype=cvips.

Pomogaeva:2007:BSP

[90] Anna Pomogaeva, Feng Long Gu, Bernard Kirtman, and Yuriko Aoki. Band structure of polymer extracted from oligomer calculations. In Simos and Maroulis [413], pages 118–121. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000118000001&idtype=cvips.

Takami:2007:MPE

[91] Toshiya Takami, Jun Maki, Jun'ichi Ooba, Yuuichi Inadomi, Hiroaki Honda, Ryutaro Susukita, Koji Inoue, Taizo Kobayashi, Rie Nogita, and Mutsumi Aoyagi. Multiphysics extension of OpenFMO framework. In Simos and Maroulis [413], pages 122–125. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000122000001&idtype=cvips.

Taube:2007:CEF

[92] Andrew G. Taube and Rodney J. Bartlett. ΛCCSD(T) energies and forces: Improving upon CCSD(T). In Simos and Maroulis [413], pages 126–129. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000126000001&idtype=cvips.

Liu:2007:ICB

[93] Kai Liu, Changhua Luo, Yanliang Ren, Jian Wan, and Xin Xu. Implementation of CCNUGrid-based computational environment for molecular modeling. In Simos and Maroulis [413], pages 130–134. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000130000001&idtype=cvips.

Harris:2007:NYO

[94] Frank E. Harris and John R. Sabin. The Nils Yngve Öhrn Symposium. In Simos and Maroulis [413], page 137. . URL http://proceedings.aip.org/getpdf/servlet/

GetPDFServlet?filetype=pdf&id=APCPCS000963000002000137000001&idtype=cvips.

Harris:2007:DCT

[95] Frank E. Harris and John R. Sabin. On a dynamic career: A tribute to Nils Yngve Öhrn. In Simos and Maroulis [413], pages 138–146. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000138000001&idtype=cvips.

Andre:2007:QCN

[96] J.-M. André, M.-Cl. André, J. G. Fripiat, and C. Lambert. Quantum chemistry and non-equilibrium thermodynamics: Does chaos play a role in quantum chemical calculations? In Simos and Maroulis [413], pages 147–150. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000147000001&idtype=cvips.

Gokhberg:2007:MPC

[97] K. Gokhberg, V. Averbukh, V. Vysotskiy, and L. S. Cederbaum. Molecular photoionization cross-sections by application of Stieltjes imaging to Lanczos pseudospectra. In Simos and Maroulis [413], pages 151–154. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000151000001&idtype=cvips.

Beebe:2007:NDF

[98] Nelson H. F. Beebe. New directions in floating-point arithmetic. In Simos and Maroulis [413], pages 155–158. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000155000001&idtype=cvips.

Brandas:2007:RQM

[99] Erkki J. Brändas. Relativity and quantum mechanics. In Simos and Maroulis [413], pages 159–162. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000159000001&idtype=cvips.

Stoyanova:2007:MEB

[100] A. Stoyanova, C. de Graaf, and R. Broer. Many-electron bands in transition metal compounds. In Simos and Maroulis [413], pages 163–166. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000163000001&idtype=cvips.

Champagne:2007:COS

[101] Benoît Champagne. Computing oscillator strengths and related properties. In Simos and Maroulis [413], pages 167–170. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000167000001&idtype=cvips.

Corongiu:2007:HFH

[102] Giorgina Corongiu and Enrico Clementi. The Hartree–Fock–Heitler–London method with applications to first and second row diatomic hydrides and homopolar molecules. In Simos and Maroulis [413], pages 171–174. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000171000001&idtype=cvips.

Cruz:2007:GSE

[103] Salvador A. Cruz, Eugenio Ley-Koo, and Remigio Cabrera-Trujillo. Ground state energy shift of He and He^{+} close to a surface: A confinement model. In Simos and Maroulis [413], pages 175–178. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000175000001&idtype=cvips`.

Fripiat:2007:FRM

[104] J. G. Fripiat, J. Delhalle, and Frank E. Harris. Fourier representation methods for Møller–Plesset perturbation theory in one-dimensionally periodic systems. In Simos and Maroulis [413], pages 179–182. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000179000001&idtype=cvips`.

Benedikt:2007:OBS

[105] Udo Benedikt, Alexander A. Auer, and Frank Jensen. Optimized basis sets for calculating spin-spin coupling constants. In Simos and Maroulis [413], pages 183–186. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000183000001&idtype=cvips`.

Dahle:2007:EEC

[106] Pål Dahle, Trygve Helgaker, Dan Jonsson, and Peter R. Taylor. Explicit electron correlation by a combined use of Gaussian-Type Orbitals and Gaussian-Type Geminals. In Simos and Maroulis [413], pages 187–190. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000187000001&idtype=cvips`.

Jensen:2007:CEP

[107] Hans Jørgen Aagaard Jensen. Can electron propagator methods be used to improve polarization propagator methods? In Simos and Maroulis [413], pages 191–192. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000191000001&idtype=cvips`.

Hoggan:2007:TWQ

[108] Philip E. Hoggan. Trial wavefunctions for quantum Monte Carlo simulations with numerically stable analytical gradients over exponential type orbitals. In Simos and Maroulis [413], pages 193–196. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000193000001&idtype=cvips`.

Kaijser:2007:TQL

[109] Per Kaijser. Three quantum leaps in the development of information security. In Simos and Maroulis [413], pages 197–199. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000197000001&idtype=cvips`.

Kirtman:2007:VPA

[110] Bernard Kirtman and Michael Springborg. Vector potential approach for response of infinite periodic systems to electric fields. In Simos and Maroulis [413], pages 200–205. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000200000001&idtype=cvips`.

Karpfen:2007:CMS

[111] Alfred Karpfen and Eugene S. Kryachko. The concept of molecular shape response quantified within force field approach. In Simos and Maroulis [413], pages 206–209.

. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000206000001&idtype=cvips.

Aspuru-Guzik:2007:RDQ

[112] Alan Aspuru-Guzik, Brian Austin, Dominik Domin, Peter T. A. Galek, Nicholas Handy, Rajendra Prasad, Romelia Salomon-Ferrer, Naoto Umezawa, and William A. Lester, Jr. Recent developments in quantum Monte Carlo: Methods and applications. In Simos and Maroulis [413], pages 210–211. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000210000001&idtype=cvips.

Linderberg:2007:SYO

[113] Jan Linderberg. The science of Yngve Öhrn. In Simos and Maroulis [413], pages 212–215. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000212000001&idtype=cvips.

Malinovskaya:2007:CPA

[114] Svetlana A. Malinovskaya. Chirped pulse adiabatic passage in CARS for imaging of biological structure and dynamics. In Simos and Maroulis [413], pages 216–218. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000216000001&idtype=cvips.

Hudock:2007:FPD

[115] Hanneli R. Hudock, Benjamin G. Levine, Alexis L. Thompson, and Todd J. Martinez. First principles dynamics of photoexcited DNA and RNA bases. In Simos and Maroulis [413], pages 219–222. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000219000001&idtype=cvips.

Rehman:2007:TPC

[116] M. Rehman, L. Olsen, and K. V. Mikkelsen. Two-photon cross-sections of photosensitizers in vacuum, in solution and within proteins. In Simos and Maroulis [413], pages 223–226. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000223000001&idtype=cvips.

Sarma:2007:LCP

[117] Manabendra Sarma, Raman K. Singh, and Manoj K. Mishra. Local complex potential based time dependent wave packet approach to calculation of vibrational excitation cross-sections in e–N_2, e–H_2 and e–CO scattering. In Simos and Maroulis [413], pages 227–230. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000227000001&idtype=cvips.

Mitin:2007:ADE

[118] Alexander V. Mitin. Accurate dissociation energies of He_2 and Be_2 calculated by MRCI method. In Simos and Maroulis [413], pages 231–234. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000231000001&idtype=cvips.

Mujica:2007:NAE

[119] Vladimiro Mujica, Thorsten Hansen, and Mark A. Ratner. Non-adiabatic effects in electron tunneling in molecular junctions. In Simos and Maroulis [413], pages 235–237. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000235000001&idtype=cvips.

Ortiz:2007:EPT

[120] J. V. Ortiz. Electron propagator theory and the development of chemical intuition. In Simos and Maroulis [413], pages 238–240. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000238000001&idtype=cvips`.

Patterson:2007:QOE

[121] Charles H. Patterson and S. Galamić-Mulaomerović. Quasiparticle and optical excitations in solid Ne and Ar: *GW* and *bse* approximations. In Simos and Maroulis [413], pages 241–244. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000241000001&idtype=cvips`.

Quack:2007:RRQ

[122] Martin Quack. Recent results in quantum chemical kinetics from high resolution spectroscopy. In Simos and Maroulis [413], pages 245–248. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000245000001&idtype=cvips`.

Rabitz:2007:WDC

[123] Herschel Rabitz. Why does controlling quantum phenomena appear easy to achieve? In Simos and Maroulis [413], pages 249–251. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000249000001&idtype=cvips`.

Matveev:2007:RGD

[124] Alexei V. Matveev and Notker Rösch. Response to geometric distortions from atom-based relativistic projection on electronic states. In Simos and Maroulis [413], pages 252–255. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000252000001&idtype=cvips`.

Simons:2007:HDL

[125] Jack Simons. How do low-energy (0.1–2 eV) electrons cause DNA strand breaks? In Simos and Maroulis [413], pages 256–259. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000256000001&idtype=cvips`.

Stolterfoht:2007:EIE

[126] N. Stolterfoht, R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, R. Hoekstra, and J. R. Sabin. Enormous isotope effects on charge transfer in slow collisions of He^{2+} with H, D, and T. In Simos and Maroulis [413], pages 260–263. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000260000001&idtype=cvips`.

Temme:2007:LRW

[127] F. P. Temme. Limitations of Racah–Wigner algebra in S_n-invariant theoretic modelling of NMR spin dynamics via dual tensorial sets. In Simos and Maroulis [413], pages 264–268. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000264000001&idtype=cvips`.

Gonzalez:2007:CSC

[128] Olmo González, Manuel Combes, Cristian Gleason, G. Hinojosa, and R. Cabrera-Trujillo. Cross sections for C^+ and O^+ production in the collision of CO_2^+ ions with atomic He. In Simos and Maroulis [413], pages 269–273. .

URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000269000001&idtype=cvips.

Voloshina:2007:ECE

[129] Elena Voloshina and Beate Paulus. Electron-correlation effects in metals from first principles: a multi-reference incremental scheme. In Simos and Maroulis [413], pages 274–277. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000274000001&idtype=cvips.

Zheng:2007:LDE

[130] Xuehe Zheng, Ngan M. Ly, and Alexei A. Stuchebrukhov. Long-distance electron transfer coupled to proton pumping and energy transduction in biological systems: A semiempirical first-principles approach. In Simos and Maroulis [413], pages 278–281. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000278000001&idtype=cvips.

Castet:2007:MSSb

[131] Frédéric Castet, Benoît Champagne, Masayoshi Nakano, and Hideaki Takahashi. Multiscale simulations for materials and life sciences. In Simos and Maroulis [413], pages 285–286. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000285000001&idtype=cvips.

Aiga:2007:DFT

[132] Fumihiko Aiga, Hiroki Iwanaga, and Akio Amano. Density functional theory investigation of Eu(III) complexes for fluorescence compounds. In Simos and Maroulis [413], pages 287–290. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000287000001&idtype=cvips.

Calzado:2007:ADH

[133] Carmen J. Calzado, Jean-Paul Malrieu, and Daniel Maynau. Approaches to dealing with high-sized polynuclear systems with *ab initio* methods. In Simos and Maroulis [413], pages 291–294. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000291000001&idtype=cvips.

Aurel:2007:VBM

[134] Philippe Aurel, Alain Fritsch, Laurent Ducasse, Mathieu Linares, Jérôme Cornil, David Beljonne, and Frédéric Castet. A valence bond model to evaluate electronic parameters for charge transport in organic aggregates. In Simos and Maroulis [413], pages 295–298. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000295000001&idtype=cvips.

Curutchet:2007:TBV

[135] Carles Curutchet, Vincenzo Russo, and Benedetta Mennucci. Through-bond versus through-space contributions on excitation energy transfer in condensed phase. In Simos and Maroulis [413], pages 299–302. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000299000001&idtype=cvips.

Dive:2007:AQC

[136] Georges Dive and Dominique Dehareng. Applied quantum chemistry to design antibiotics. In Simos and Maroulis [413], pages 303–305. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000303000001&idtype=cvips.

Ehara:2007:POL

[137] Masahiro Ehara and Hiroshi Nakatsuji. Photochemistry of organic light-emitting diodes. In Simos and Maroulis [413], pages 306–310. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000306000001&idtype=cvips`.

Fukunishi:2007:SBD

[138] Yoshifumi Fukunishi. Structure-based drug screening and ligand-based drug screening toward protein-compound network. In Simos and Maroulis [413], pages 311–314. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000311000001&idtype=cvips`.

Guallar:2007:QMS

[139] Victor Guallar. QMMM methods for the spin density in heme compound I. In Simos and Maroulis [413], pages 315–317. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000315000001&idtype=cvips`.

Guthmuller:2007:NOP

[140] J. Guthmuller and D. Simon. Nonlinear optical properties of conjugated molecules studied by time-dependent density functional theory. In Simos and Maroulis [413], pages 318–321. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000318000001&idtype=cvips`.

Sugiyama:2007:TSD

[141] Ayumu Sugiyama, Keigo Nishikawa, Tetsunori Yamamoto, Acep Purqon, Kiyoshi Nishikawa, and Hidemi Nagao. Theoretical studies on docking dynamics and electronic structure in metalloprotein complexes. In Simos and Maroulis [413], pages 322–325. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000322000001&idtype=cvips`.

Andreu:2007:IHD

[142] R. Andreu, M. J. Blesa, S. Franco, J. Garín, and J. Orduna. *Ab Initio* HF and DFT calculation of the second order NLO response of tetrathiafulvalene and 1,3-dithiole derivatives. In Simos and Maroulis [413], pages 326–329. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000326000001&idtype=cvips`.

Luis:2007:TVI

[143] Josep M. Luis, Miquel Torrent-Sucarrat, Ove Christiansen, and Bernard Kirtman. Treatment of vibronic interactions using variational methods for nuclear motion. In Simos and Maroulis [413], pages 330–333. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000330000001&idtype=cvips`.

Kitagawa:2007:GOS

[144] Y. Kitagawa, T. Saito, Y. Nakanishi, M. Ito, M. Shoji, K. Koizumi, S. Yamanaka, T. Kawakami, M. Okumura, and K. Yamaguchi. Geometry optimization without spin contamination error — approximately spin projected optimization method. In Simos and Maroulis [413], pages 334–337. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000334000001&idtype=cvips`.

Kobayashi:2007:ISU

[145] Takao Kobayashi, Motoyuki Shiga, Akinori Murakami, and Shinichiro Nakamura. *Ab initio* study of ultrafast photochemical ring-opening reaction of 1,3-cyclohexadiene. In Simos and Maroulis [413], pages 338–341. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000338000001&idtype=cvips`.

Matubayasi:2007:FES

[146] Nobuyuki Matubayasi. Free energy of solvation in the energetic perspective. In Simos and Maroulis [413], pages 342–345. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000342000001&idtype=cvips`.

Mennucci:2007:HME

[147] Benedetta Mennucci, Carles Curutchet, Roberto Cammi, and Gregory D. Scholes. How the molecular environment controls excitation energy transfer and light harvesting: a quantum mechanical model. In Simos and Maroulis [413], pages 346–349. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000346000001&idtype=cvips`.

Mikkelsen:2007:TMS

[148] Kurt V. Mikkelsen. Theoretical methods for structured environments. In Simos and Maroulis [413], pages 350–354. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000350000001&idtype=cvips`.

Zdetsis:2007:SP

[149] Aristides Zdetsis. Symposium 2 preface. In Simos and Maroulis [413], pages 357–358. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000357000001&idtype=cvips`.

Magri:2007:CGN

[150] Rita Magri, F. Iori, E. Degoli, O. Pulci, and S. Ossicini. Codoping goes nano: Structural and optical properties of boron and phosphorus codoped silicon nanocrystals. In Simos and Maroulis [413], pages 359–362. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000359000001&idtype=cvips`.

Kulkova:2007:IIS

[151] Svetlana E. Kulkova, Sergey S. Kulkov, Sergey V. Eremeev, and Dmitry I. Bazhanov. Ab-initio investigations of surface electronic structure and metal-hydrogen interaction in titanium- and palladium-based alloys. In Simos and Maroulis [413], pages 363–366. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000363000001&idtype=cvips`.

Baranek:2007:TSS

[152] Ph. Baranek, L. Gauthier, and M. Marrony. Theoretical study of sulphur interaction with ceria. In Simos and Maroulis [413], pages 367–370. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000367000001&idtype=cvips`.

Patterson:2007:ESV

[153] Charles H. Patterson and Andrew D. Rowan. Electronic structure and vibrational spectra of magnetite. In Simos and Maroulis [413], pages 371–374. .

URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000371000001&idtype=cvips.

Koukaras:2007:HSF

[154] E. N. Koukaras, A. D. Zdetsis, and C. S. Garoufalis. High-stability finite-length silicon nanowires: A real space theoretical study. In Simos and Maroulis [413], pages 375–378. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000375000001&idtype=cvips.

Baranek:2007:PDP

[155] Ph. Baranek. Pressure driven phase transitions of ferroelectric KNb_3: A hybrid functional approach. In Simos and Maroulis [413], pages 379–382. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000379000001&idtype=cvips.

Zdetsis:2007:AFK

[156] Aristides D. Zdetsis. Is aromaticity and fluxionality the key to magicity of Si_6 cluster? In Simos and Maroulis [413], pages 383–386. . URL http://www.springer.com/physics/atoms/book/978-0-7354-0478-6.

Eremeev:2007:IES

[157] S. V. Eremeev, S. E. Kulkova, and I. Yu. Smolin. Investigation of the electronic structure and magnetic properties of Heusler half-metallic alloys at surfaces and interfaces. In Simos and Maroulis [413], pages 387–390. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000387000001&idtype=cvips.

Baranek:2007:RIV

[158] Ph. Baranek and M. Marrony. Raman and infrared vibrational properties of the protonic defect in the $BaMO_3$ (M = Zr, Ce) perovskites: a quantum mechanical study of protonic diffusion mechanisms. In Simos and Maroulis [413], pages 391–394. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000391000001&idtype=cvips.

Koukaras:2007:ESP

[159] Emmanuel N. Koukaras and Aristides D. Zdetsis. Electronic and structural properties of $M@Si_{12}$ and $M@Si_{12}H_{12}$ clusters, M = Ni, Zn. In Simos and Maroulis [413], pages 395–398. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000395000001&idtype=cvips.

Bitsanis:2007:SCM

[160] Ioannis A. Bitsanis and Evangelos Manias. Symposium 3: Computational methods in chemical engineering: Physical chemistry. In Simos and Maroulis [413], pages 401–403. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000401000001&idtype=cvips.

Decterov:2007:MVA

[161] Sergei A. Decterov, A. Nicholas Grundy, In-Ho Jung, and Arthur D. Pelton. Modeling the viscosity of aluminosilicate melts. In Simos and Maroulis [413], pages 404–407. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000404000001&idtype=cvips.

Makrodimitri:2007:MMP

[162] Zoi A. Makrodimitri and Ioannis G. Economou. Molecular modeling of polydimethylsiloxane mixtures. In Simos and Maroulis [413], pages 408–411. .

URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000408000001&idtype=cvips.

Verros:2007:PCC

[163] G. D. Verros, T. Latsos, K. E. Anagnostou, P. Avlakiotis, C. Chaikalis, C. Liolios, D. Antoniou, S. Kotsopoulos, and P. Arsenos. Physico-chemical characteristics of thermopylae natural hot water springs in central Greece: Chemical geothermometry. In Simos and Maroulis [413], pages 412–415. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000412000001&idtype=cvips.

Khokhlov:2007:CDCb

[164] Alexei R. Khokhlov, Yury A. Kriksin, Igor Ya. Erukhimovich, and Pavel G. Khalatur. Computer design of copolymers with desired functionalities: Microphase separation in diblock copolymers with amphiphilic block. In Simos and Maroulis [413], pages 416–422. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000416000001&idtype=cvips.

Efthymiopoulos:2007:CPD

[165] Pavlos Efthymiopoulos and Marios Kosmas. Conformational properties of dendritic homopolymers with interacting branching points. In Simos and Maroulis [413], pages 423–427. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000423000001&idtype=cvips.

Rissanou:2007:CTM

[166] A. N. Rissanou, S. H. Anastasiadis, and I. A. Bitsanis. Conformational transitions of a model polymeric system near attractive surfaces: a Monte Carlo study. In Simos and Maroulis [413], pages 428–431. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000428000001&idtype=cvips.

Sheka:2007:OEN

[167] Elena F. Sheka. Odd electrons of nanomaterials: A new approach to computational chemical engineering. In Simos and Maroulis [413], pages 432–435. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000432000001&idtype=cvips.

Kritikos:2007:TSA

[168] Georgios Kritikos and Andreas F. Terzis. Theoretical study of adsorption of star-polymers by mean field theory. In Simos and Maroulis [413], pages 436–439. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000436000001&idtype=cvips.

Verros:2007:VGR

[169] George D. Verros. On the validity of the geometric rule in multi-component diffusion. In Simos and Maroulis [413], pages 440–443. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000440000001&idtype=cvips.

Yiannourakou:2007:PEC

[170] Marianna Yiannourakou, Ioannis Bitsanis, and Ioannis Economou. Phase equilibrium of colloid systems with particle size dispersity: a Monte Carlo study. In Simos and Maroulis [413], pages 444–447. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000444000001&idtype=cvips.

Yiannourakou:2007:CPE

[171] Marianna Yiannourakou, Luca Marsella, Frédérick de Meyer, and Berend Smit. Clustering of proteins embedded in lipid bilayers: a Monte Carlo study. In Simos and Maroulis [413], pages 448–451. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000448000001&idtype=cvips`.

Bieniasz:2007:PIS

[172] L. K. Bieniasz and D. Britz. Preface: International Symposium on Computational Electrochemistry. In Simos and Maroulis [413], pages 455–456. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000455000001&idtype=cvips`.

Baronas:2007:CMA

[173] Romas Baronas, Feliksas Ivanauskas, and Juozas Kulys. Computational modelling of amperometric enzyme electrodes with selective and perforated membranes. In Simos and Maroulis [413], pages 457–460. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000457000001&idtype=cvips`.

Jakubowska:2007:SPD

[174] M. Jakubowska, B. Ba, E. Niewiara, W. Reczyński, and W. W. Kubiak. Signal processing in DP and NP voltammetry by means of a dedicated mother wavelet. In Simos and Maroulis [413], pages 461–464. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000461000001&idtype=cvips`.

Bozzini:2007:TIE

[175] Benedetto Bozzini, Deborah Lacitignola, and Ivonne Sgura. Turing instability in an electrodeposition morphogenesis model: An analytical, numerical and experimental study. In Simos and Maroulis [413], pages 465–468. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000465000001&idtype=cvips`.

Carvalho:2007:UDS

[176] R. H. Carvalho, M. A. N. D. A. Lemos, F. Lemos, and F. Ramôa Ribeiro. Using digital simulation to study hydroquinone oxidation on porous electrodes by cyclic voltammetry. In Simos and Maroulis [413], pages 469–472. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000469000001&idtype=cvips`.

Filipek:2007:NMA

[177] R. Filipek, K. Szyszkiewicz, M. Danielewski, and A. Lewenstam. Numerical method and analysis of consistency for electrodiffusion problem. In Simos and Maroulis [413], pages 473–476. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000473000001&idtype=cvips`.

Daasbjerg:2007:ITS

[178] Kim Daasbjerg, Umberto Del Pennino, Valentina De Renzi, Claudio Fontanesi, Francesca Parenti, and Augusto Rastelli. An ab-initio theoretical study of the electrochemical grafting process of alkynil(aryl)iodonium salts on glassy carbon surfaces. In Simos and Maroulis [413], pages 477–480. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000477000001&idtype=cvips`.

Minami:2007:CSI

[179] Yusuke Minami and Albert J. Fry. Computational study of the interactions between electrochemically-generated 1,4-dinitrobenzene dianion and substituted imidazolium ions. In Simos and Maroulis [413], pages 481–484. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000481000001&idtype=cvips.

Nechaev:2007:QCS

[180] I. Nechaev, A. Vvedenskii, and S. Grushevskaya. Quantum chemical study of Cl^- anion adsorption on low-index faces of Cu, Ag and Au from aqueous solutions. In Simos and Maroulis [413], pages 485–487. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000485000001&idtype=cvips.

Nechaev:2007:ESF

[181] I. Nechaev, V. Sokova, A. Vvedenskii, and S. Grushevskaya. Electronic structure of five-atomic thickness Cu, Ag, Au and Pd films with adsorbed chloride anion. In Simos and Maroulis [413], pages 488–490. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000488000001&idtype=cvips.

Ryan:2007:UFA

[182] Michael D. Ryan and Robert L. Keesey. Use of factor analysis in multi-electron spectroelectrochemistry. In Simos and Maroulis [413], pages 491–494. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000491000001&idtype=cvips.

Uudsemaa:2007:IAC

[183] Merle Uudsemaa and Toomas Tamm. Inclusion of additional coordination sphere into cluster-model redox potential calculations. In Simos and Maroulis [413], pages 495–499. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000495000001&idtype=cvips.

Trauble:2007:NBC

[184] Markus Träuble, Carolina Nunes Kirchner, and Gunther Wittstock. Nonlinear boundary conditions in simulations of electrochemical experiments using the boundary element method. In Simos and Maroulis [413], pages 500–503. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000500000001&idtype=cvips.

VanDamme:2007:NSM

[185] S. Van Damme and J. Deconinck. Numerical simulation of mass transport in electrochemical systems based on the mean spherical approximation. In Simos and Maroulis [413], pages 504–507. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000504000001&idtype=cvips.

Nikolic:2007:PSM

[186] Sonja Nikolić. Preface of the 5^{th} symposium on mathematical chemistry. In Simos and Maroulis [413], pages 511–512. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000511000001&idtype=cvips.

Mezey:2007:DCT

[187] Paul G. Mezey. On discrete to continuum transformations and the universal molecule model — A mathematical chemistry perspective of molecular families. In Simos and Maroulis [413], pages 513–516. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000513000001&idtype=cvips.

Fowler:2007:EGM

[188] P. W. Fowler. Energies of graphs and molecules. In Simos and Maroulis [413], pages 517–520. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000517000001&idtype=cvips.

Basic:2007:MAH

[189] Ivan Basic, Damir Nadramija, Mario Flajslik, Dragan Amić, and Bono Lucić. Modeling anti-HIV activity of HEPT derivatives revisited. multiregression models are not inferior ones. In Simos and Maroulis [413], pages 521–523. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000521000001&idtype=cvips.

Janezic:2007:MMN

[190] Dusanka Janezic, Janez Konc, Matej Praprotnik, Matej Penca, and Ksenija Poljanec. Molecular modeling — A new approach. In Simos and Maroulis [413], pages 524–527. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000524000001&idtype=cvips.

Iliev:2007:SIL

[191] Valentin Vankov Iliev. On some isomers of the linear alkanes. In Simos and Maroulis [413], pages 528–531. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000528000001&idtype=cvips.

Krygowski:2007:AWD

[192] Tadeusz M. Krygowski and Halina Szatyłowicz. Aromaticity — what does it mean? In Simos and Maroulis [413], pages 532–535. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000532000001&idtype=cvips.

Pipek:2007:QMO

[193] János Pipek. Quantum mechanical operators in multiresolution Hilbert spaces. In Simos and Maroulis [413], pages 536–539. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000536000001&idtype=cvips.

Pogliani:2007:ONC

[194] Lionello Pogliani. Old and new concepts in chemical graph theory. In Simos and Maroulis [413], pages 540–543. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000540000001&idtype=cvips.

Basak:2007:QCF

[195] Subhash C. Basak, Brian D. Gute, and Gregory D. Grunwald. Quantitative comparison of five molecular structure spaces in selecting analogs of chemicals. In Simos and Maroulis [413], pages 544–547. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000544000001&idtype=cvips.

Basak:2007:PSM

[196] Subhash C. Basak, Denise Mills, Douglas M. Hawkins, and Jessica J. Kraker. Proper statistical modeling and validation in QSAR: A case study in the prediction of rat fat-air partitioning. In Simos and Maroulis [413], pages 548–551. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000548000001&idtype=cvips.

Jako:2007:GBD

[197] Éena Jakó. Generalized Boolean descriptors for biological macromolecules. In Simos and Maroulis [413], pages 552–554. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000552000001&idtype=cvips.

Kim:2007:SAM

[198] Tai-Hoon Kim. Symposium 6: Approaches and methods of security engineering. In Simos and Maroulis [413], page 557. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000557000001&idtype=cvips.

Lee:2007:HPM

[199] Dong-Young Lee and Minsoo Kim. Hierarchical policy model for managing heterogeneous security systems. In Simos and Maroulis [413], pages 558–562. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000558000001&idtype=cvips.

Song:2007:RBC

[200] Jae-Gu Song, Gil-Cheol Park, and Seoksoo Kim. RFID based context information security system architecture for securing personal information under ubiquitous environment. In Simos and Maroulis [413], pages 563–566. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000563000001&idtype=cvips.

Kim:2007:AAR

[201] Wankyung Kim and Wooyoung Soh. Applying association rule of the data mining method for the network event analysis. In Simos and Maroulis [413], pages 567–570. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000567000001&idtype=cvips.

Ko:2007:SRT

[202] Hoon Ko, Jiyeon Kim, Jongjin Jung, Susan Joe, Yongjun Lee, and Yoonseok Chang. A study on the RFID tag encryption using fast SEED. In Simos and Maroulis [413], pages 571–574. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000571000001&idtype=cvips.

Kim:2007:MOB

[203] Jiyeon Kim, Jongjin Jung, Ukjae Ryu, Hoon Ko, Susan Joe, Yongjun Lee, Boyeon Kim, Yunseok Chang, and Kyoonha Lee. Multiple object based RFID system using security level. In Simos and Maroulis [413], pages 575–578. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000575000001&idtype=cvips.

Garavelli:2007:MCM

[204] Marco Garavelli. Modelling complex molecular and biomaterial systems: Simulation of reactive processes, methodological advances and interplay with the experiments. In

Simos and Maroulis [413], pages 581–582. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000581000001&idtype=cvips`.

Bearpark:2007:CCE

[205] Michael J. Bearpark, Francois Ogliaro, Thom Vreven, Martial Boggio-Pasqua, Michael J. Frisch, Susan M. Larkin, and Michael A. Robb. CASSCF calculations for excited states of large molecules: Choosing when to use the RASSCF, ONIOM and MMVB approximations. In Simos and Maroulis [413], pages 583–585. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000583000001&idtype=cvips`.

Blancafort:2007:BDE

[206] Lluís Blancafort, David Asturiol, Annapaola Migani, Monika Kobyłecka, and Janusz Rak. Benign and degrading excited-state processes of DNA nucleobases and their derivatives. In Simos and Maroulis [413], pages 586–588. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000586000001&idtype=cvips`.

Buma:2007:MSF

[207] Wybren Jan Buma, Mattijs de Groot, and Anouk M. Rijs. Molecular structure and function probed by high-resolution spectroscopy. In Simos and Maroulis [413], pages 589–592. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000589000001&idtype=cvips`.

Carloni:2007:MSS

[208] Paolo Carloni. Molecular simulation studies of proteins involved in parkinson's disease. In Simos and Maroulis [413], page 593. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000593000001&idtype=cvips`.

Castano:2007:RIS

[209] Obis Castaño, Unai Sancho, Marco Garavelli, Massimo Olivucci, and Luis Manuel Frutos. The role of intersection space segments in photochemical reactions. In Simos and Maroulis [413], pages 594–597. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000594000001&idtype=cvips`.

Cavalli:2007:PCP

[210] Andrea Cavalli, Anna Berteotti, Davide Branduardi, Francesco L. Gervasio, Maurizio Recanatini, and Michele Parrinello. Protein conformational plasticity: the "off-on" switching movement in Cdk5. In Simos and Maroulis [413], page 598. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000598000001&idtype=cvips`.

Cimiraglia:2007:CCE

[211] Renzo Cimiraglia and Celestino Angeli. The calculation of the correlation energy in ground and excited states: the n-electron valence state perturbation theory approach. In Simos and Maroulis [413], pages 599–602. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000599000001&idtype=cvips`.

Semeraro:2007:AMD

[212] Monica Semeraro, Serena Silvi, and Alberto Credi. Artificial molecular devices and machines driven by light. In Simos and Maroulis [413], pages 603–606.

. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000603000001&idtype=cvips.

Crespo-Hernandez:2007:VSE

[213] Carlos E. Crespo-Hernández and Christopher N. J. Marai. Vertical singlet excitations on adenine dimer: A time dependent density functional study. In Simos and Maroulis [413], pages 607–610. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000607000001&idtype=cvips.

Danos:2007:AMC

[214] Vincent Danos. Agile modelling of cellular signalling. In Simos and Maroulis [413], pages 611–614. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000611000001&idtype=cvips.

Elisei:2007:KSI

[215] Fausto Elisei, Arianna Barbafina, Benedetta Carlotti, and Loredana Latterini. Kinetic and spectroscopic investigations by ultrafast absorption and emission techniques. In Simos and Maroulis [413], pages 615–618. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000615000001&idtype=cvips.

Feret:2007:RAB

[216] Jérôme Feret. Reachability analysis of biological signalling pathways by abstract interpretation. In Simos and Maroulis [413], pages 619–622. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000619000001&idtype=cvips.

Frutos:2007:NCA

[217] Luis Manuel Frutos, A. Ulises Acuña, and Obis Castaño. New computational approaches in the study of *nonvertical* triplet energy transfer. In Simos and Maroulis [413], pages 623–626. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000623000001&idtype=cvips.

Fuss:2007:BME

[218] Werner Fuß. Branching and momentum effects in photochemistry. In Simos and Maroulis [413], pages 627–630. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000627000001&idtype=cvips.

Santoro:2007:TUE

[219] Fabrizio Santoro, T. Gustavsson, Sandro Lami, Vincenzo Barone, and Roberto Improta. Towards the understanding of the excited state dynamics of nucleic acids: Solvent and stacking effect on the photophysical behavior of nucleobases. In Simos and Maroulis [413], pages 631–634. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000631000001&idtype=cvips.

Kandori:2007:DLE

[220] Hideki Kandori. The determinant of light-energy and light-signal conversion in rhodopsins. In Simos and Maroulis [413], pages 635–637. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000635000001&idtype=cvips.

Krivine:2007:ESS

[221] Jean Krivine. An exact and scalable stochastic simulation algorithm. In Simos and Maroulis [413], pages 638–641. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000638000001&idtype=cvips.

Mardare:2007:CMS

[222] Radu Mardare and Adaoha Ihekwaba. A calculus for modelling, simulating and analysing compartmentalized biological systems. In Simos and Maroulis [413], pages 642–646. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000642000001&idtype=cvips.

Negri:2007:FMM

[223] Fabrizia Negri. Functional molecular materials: Modelling structure, optical properties, intermolecular interactions. In Simos and Maroulis [413], pages 647–650. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000647000001&idtype=cvips.

Lago:2007:SOW

[224] N. Faginas Lago, M. Paolantoni, A. Laganá, and M. Alberti. Structural order in water: Comparison between the spectral analysis of Raman data and molecular dynamics results. In Simos and Maroulis [413], pages 651–654. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000651000001&idtype=cvips.

Conti:2007:ISD

[225] Irene Conti, Marco Garavelli, and Giorgio Orlandi. An *ab initio* study of decay mechanism of adenine: the facile path of the amino NH bond cleavage. In Simos and Maroulis [413], pages 655–658. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000655000001&idtype=cvips.

Ravaglia:2007:ICT

[226] Marcella Ravaglia, Marco Garavelli, Matthew Polson, and Franco Scandola. Iridium complexes with terdentate ligands: Cyclometalated vs. polypyridine analogues; hybrid vs. "pure" DFT. In Simos and Maroulis [413], pages 659–662. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000659000001&idtype=cvips.

Bismuth:2007:PER

[227] O. Bismuth, A. Kahan, N. Friedman, M. Sheves, and S. Ruhman. Primary events in retinal proteins revealed by ultrafast spectroscopy. In Simos and Maroulis [413], pages 663–666. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000663000001&idtype=cvips.

Santoro:2007:QDU

[228] Fabrizio Santoro, Vincenzo Barone, Roberto Improta, Alessandro Lami, and Massimo Olivucci. Quantum dynamics of ultrafast photoinduced processes in biological molecules. In Simos and Maroulis [413], pages 667–670. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000667000001&idtype=cvips.

Shibata:2007:FSI

[229] Mikihiro Shibata and Hideki Kandori. FTIR studies of internal water molecules of bacteriorhodopsin: Structural analysis of halide-bound D85S and D212N mu-

tants in the Schiff base region. In Simos and Maroulis [413], pages 671–673. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000671000001&idtype=cvips.

Skourtis:2007:FCT

[230] Spiros S. Skourtis, Tatiana Prytkova, and David N. Beratan. Flavin charge transfer transitions assist DNA photolyase electron transfer. In Simos and Maroulis [413], pages 674–677. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000674000001&idtype=cvips.

Weingart:2007:PIT

[231] Oliver Weingart and Volker Buss. Protein induced torsion of the retinal chromophore and how it affects the photochemistry of rhopdopsin. In Simos and Maroulis [413], pages 678–680. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000678000001&idtype=cvips.

Zavattaro:2007:CVM

[232] Gianluigi Zavattaro. Compositional vs. monolithical modeling of nano devices. In Simos and Maroulis [413], pages 681–684. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000681000001&idtype=cvips.

Altoe:2007:CPT

[233] Piero Altoè, Marco Stenta, Andrea Bottoni, and Marco Garavelli. COBRAMM (part 1): a tunable QM/MM approach to chemical reactivity, structure and physicochemical properties prediction. In Simos and Maroulis [413], pages 685–688. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000685000001&idtype=cvips.

Altoe:2007:RGC

[234] Piero Altoè, Marco Stenta, and Marco Garavelli. Rhodopsin and GFP chromophores: QM/MM absorption spectra in solvent and protein. In Simos and Maroulis [413], pages 689–692. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000689000001&idtype=cvips.

DeFusco:2007:CTP

[235] Giulia C. De Fusco, Piero Altoè, and Marco Garavelli. The CIS–TRANS photoisomerization of the phytochromobilin. In Simos and Maroulis [413], pages 693–695. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000693000001&idtype=cvips.

Calvaresi:2007:CQM

[236] Matteo Calvaresi, Marco Stenta, Piero Altoè, Andrea Bottoni, Marco Garavelli, and Domenico Spinelli. Computational QM/MM study of the reaction mechanism of *Human Glutathione S-Transferase A3-3*. In Simos and Maroulis [413], pages 696–698. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000696000001&idtype=cvips.

Conti:2007:ACT

[237] Irene Conti, Marco Garavelli, and Giorgio Orlandi. Azobenzene cis–trans photoisomerization mechanism: Characterization of the decay ways from the lowest. In Simos and Maroulis [413], pages 699–702. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000699000001&idtype=cvips.

Elli:2007:HCS

[238] Stefano Elli, Andrea Magrì, Elisa Venturini, Fabrizia Negri, Alessandro Abbotto, Luca Bellotto, Anna Painelli, Cristina Sissa, and Francesca Terenziani. Heteroaromatic chromophores: Structure, electric properties, condensed phase and aggregation effects: a combined experimental and theoretical study. In Simos and Maroulis [413], pages 703–705. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000703000001&idtype=cvips.

Olaso-Gonzalez:2007:UET

[239] Gloria Olaso-González, Manuela Merchán, and Luis Serrano-Andrés. Ultrafast electron transfer in photosynthesis: Reduced pheophytin and quinone interaction mediated by conical intersections. In Simos and Maroulis [413], pages 706–709. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000706000001&idtype=cvips.

Olaso-Gonzalez:2007:TUS

[240] Gloria Olaso-González, Gaia Tomasello, Piero Altoè, Marco Stenta, Luis Serrano-Andrés, Manuela Merchán, and Marco Garavelli. Toward an understanding of the spectral tuning in rhodopsin. In Simos and Maroulis [413], pages 710–712. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000710000001&idtype=cvips.

Hall:2007:TLO

[241] Katherine F. Hall, Thom Vreven, Michael J. Frisch, and Michael J. Bearpark. Three-layer ONIOM studies of rhodopsin in the dark state: Shedding light on the protonation state of Glu-181. In Simos and Maroulis [413], page 713. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000713000001&idtype=cvips.

Stenta:2007:CPO

[242] Marco Stenta, Piero Altoè, Andrea Bottoni, and Marco Garavelli. COBRAMM (part 2): an overview on some computational details; geometry optimization, frequency calculation, analysis of the results. In Simos and Maroulis [413], pages 714–716. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000714000001&idtype=cvips.

Stenta:2007:CAD

[243] Marco Stenta, Matteo Calvaresi, Piero Altoè, Domenico Spinelli, Marco Garavelli, and Andrea Bottoni. The catalytic activity of diaminopimelate epimerase: a QM/MM study. In Simos and Maroulis [413], pages 717–719. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000717000001&idtype=cvips.

Stenta:2007:CAP

[244] Marco Stenta, Matteo Calvaresi, Piero Altoè, Domenico Spinelli, Marco Garavelli, and Andrea Bottoni. The catalytic activity of proline racemase: a QM/MM study. In Simos and Maroulis [413], pages 720–723. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000720000001&idtype=cvips.

Tomasello:2007:IIM

[245] Gaia Tomasello, Piero Altoè, Marco Garavelli, and Giorgio Orlandi. Ab initio investigation to model stilbene photo-physical properties by combining CC2 topological investigation and CASPT2 energy corrections. In Simos and Maroulis [413], pages 724–726.

. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000724000001&idtype=cvips.

Tomasello:2007:RPR

[246] Gaia Tomasello, Piero Altoè, Marco Stenta, Gloria Olaso-González, Marco Garavelli, and Giorgio Orlandi. Retinal photoisomerization in rhodopsin: Electrostatic and steric catalysis. In Simos and Maroulis [413], pages 727–730. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000727000001&idtype=cvips.

Paspalakis:2007:PQC

[247] Emmanuel Paspalakis and Ioannis Thanopulos. Preface: Quantum control and light-matter interactions: Recent computational and theoretical results. In Simos and Maroulis [413], pages 733–735. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000733000001&idtype=cvips.

Angelakis:2007:IUQ

[248] Dimitris G. Angelakis and Alastair Kay. Implementing universal quantum gates in coupled cavities. In Simos and Maroulis [413], pages 736–739. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000736000001&idtype=cvips.

Boviatsis:2007:QCE

[249] John Boviatsis and Evangelos Voutsinas. Quantum control and entanglement of two electrons in a double quantum dot structure. In Simos and Maroulis [413], pages 740–743. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000740000001&idtype=cvips.

Brandao:2007:QPT

[250] F. G. S. L. Brandão, M. J. Hartmann, and M. B. Plenio. Quantum phase transitions in coupled arrays of cavities. In Simos and Maroulis [413], pages 744–747. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000744000001&idtype=cvips.

Chatzisavvas:2007:SCS

[251] K. Ch. Chatzisavvas, C. Daskaloyannis, and S. G. Schirmer. A simple control switch model for quantum computation. In Simos and Maroulis [413], pages 748–751. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000748000001&idtype=cvips.

Daniele:2007:SNM

[252] R. Daniele, G. Castiglia, P. P. Corso, E. Fiordilino, F. Morales, G. Orlando, and F. Persico. The study of the nuclear motion in ${D_2}^+$ molecular ion by using the harmonic spectra. In Simos and Maroulis [413], pages 752–755. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000752000001&idtype=cvips.

Evers:2007:QCI

[253] Jörg Evers, Martin Kiffner, and Christoph H. Keitel. Quantum control of interacting multiatom systems. In Simos and Maroulis [413], pages 756–759. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000756000001&idtype=cvips.

Ficek:2007:CQS

[254] Zbigniew Ficek. Cavity QED schemes for controlled creation of entanglement between distant atoms. In Simos and Maroulis [413], pages 760–763. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000760000001&idtype=cvips.

Garraway:2007:DRT

[255] Barry M. Garraway. Dressed rf trapping. In Simos and Maroulis [413], pages 764–767. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000764000001&idtype=cvips.

Gong:2007:CCE

[256] Shangqing Gong, Keyu Xia, and Yueping Niu. Coherent control of extreme nonlinear optical properties of quantum system via ultrashort laser pulses. In Simos and Maroulis [413], pages 768–771. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000768000001&idtype=cvips.

Guerin:2007:CAM

[257] S. Guérin. Control of atomic and molecular processes by designed external fields: From adiabatic to ultrashort pulse strategies. In Simos and Maroulis [413], pages 772–776. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000772000001&idtype=cvips.

Popsueva:2007:ESF

[258] V. Popsueva, J. P. Hansen, and J. Caillat. Electronic structure of few-electron quantum dot molecules. In Simos and Maroulis [413], pages 777–780. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000777000001&idtype=cvips.

Jin:2007:CAL

[259] Luling Jin, Shiqi Jin, and Shangqing Gong. Controllable atom localization in four-level atomic systems. In Simos and Maroulis [413], pages 781–784. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000781000001&idtype=cvips.

Ntalaperas:2007:IHG

[260] D. Ntalaperas and N. Konofaos. Implementation of a Hadamard gate using laser light on a phosphorus doped Si device. In Simos and Maroulis [413], pages 785–787. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000785000001&idtype=cvips.

Pentaris:2007:PFW

[261] D. Pentaris, N. Merlemis, A. Lyras, and T. Efthimiopoulos. Parametric four-wave mixing in low atomic densities of potassium vapor. In Simos and Maroulis [413], pages 788–791. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000788000001&idtype=cvips.

Retzker:2007:FCT

[262] A. Retzker and M. B. Plenio. Fast cooling of trapped ions using the dynamical Stark shift. In Simos and Maroulis [413], pages 792–795. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000792000001&idtype=cvips.

Schirmer:2007:IQG

[263] Sonia G. Schirmer, Gajendran Kandasamy, and Lloyd C. L. Hollenberg. Implementation of quantum gates via optimal control in the presence of cross-talk. In Simos and Maroulis [413], pages 796–800. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000796000001&idtype=cvips`.

Serrat:2007:OBT

[264] Carles Serrat and Jens Biegert. Optimal bichromatic two-photon excitation with near-resonant chirped pulses. In Simos and Maroulis [413], pages 801–804. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000801000001&idtype=cvips`.

Singh:2007:SDD

[265] Mahi R. Singh. Simulations of dipole-dipole interaction in nonlinear photonic crystals doped with nanoparticles. In Simos and Maroulis [413], pages 805–808. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000805000001&idtype=cvips`.

Skourtis:2007:MDS

[266] Spiros S. Skourtis and David N. Beratan. A molecular double slit paradigm. In Simos and Maroulis [413], pages 809–812. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000809000001&idtype=cvips`.

Sola:2007:QCM

[267] I. R. Sola, J. González-Vázquez, J. Santamaria, V. S. Malinovsky, and B. Y. Chang. Quantum control of molecular properties. In Simos and Maroulis [413], pages 813–816. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000813000001&idtype=cvips`.

Sun:2007:LSC

[268] Hui Sun, Yueping Niu, and Shangqing Gong. Large self- and cross-phase modulations via Fano interference in asymmetric quantum wells. In Simos and Maroulis [413], pages 817–820. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000817000001&idtype=cvips`.

Takami:2007:AAC

[269] Toshiya Takami and Hiroshi Fujisaki. Analytic approach for controlling realistic quantum chaotic systems. In Simos and Maroulis [413], pages 821–824. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000821000001&idtype=cvips`.

Fountoulakis:2007:CPT

[270] Antonios Fountoulakis, Andreas F. Terzis, and Emmanuel Paspalakis. Controlled population transfer in a double quantum dot system. In Simos and Maroulis [413], pages 825–828. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000825000001&idtype=cvips`.

Tognetti:2007:TCL

[271] M. V. Tognetti, R. Buffa, S. Cavalieri, L. Fini, E. Ignesti, and E. Sali. Temporal compression of laser pulses by coherent control. In Simos and Maroulis [413], pages 829–831. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000829000001&idtype=cvips`.

Ivanov:2007:SAU

[272] P. A. Ivanov and N. V. Vitanov. Synthesis of arbitrary unitary transformations in quantum systems by Householder reflections. In Simos and Maroulis [413], pages 832–835. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000832000001&idtype=cvips.

Voutsinas:2007:ICE

[273] Evangelos Voutsinas and John Boviatsis. Initial conditions effects in the population dynamics of a driven semiconductor quantum well structure. In Simos and Maroulis [413], pages 836–839. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000836000001&idtype=cvips.

Wisniacki:2007:QCU

[274] D. A. Wisniacki, G. E. Murgida, and P. I. Tamborenea. Quantum control using diabatic and adiabatic transitions. In Simos and Maroulis [413], pages 840–842. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000840000001&idtype=cvips.

Nishikawa:2007:LCP

[275] Kiyoshi Nishikawa, Kimikazu Sugimori, and Hidemi Nagao. Laser control of photoassociation in reaction O + H. In Simos and Maroulis [413], pages 843–846. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000843000001&idtype=cvips.

Batzias:2007:SIE

[276] Fragiskos Batzias. 4th Symposium on Industrial and Environmental Case Studies. In Simos and Maroulis [413], pages 849–850. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000849000001&idtype=cvips.

Anagnostopoulos:2007:UGF

[277] K. P. Anagnostopoulos and A. P. Vavatsikos. Using GIS and fuzzy logic for wastewater treatment processes site selection: The case of Rodopi prefecture. In Simos and Maroulis [413], pages 851–855. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000851000001&idtype=cvips.

Batzias:2007:FMR

[278] A. F. Batzias. Fuzzy multicriteria ranking of aluminium coating methods. In Simos and Maroulis [413], pages 856–861. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000856000001&idtype=cvips.

Batzias:2007:ASP

[279] D. F. Batzias and D. K. Sidiras. Analyte in situ processing at micro-scale for enhancing biosensor functionality — A new taxonomic/partonomic approach. In Simos and Maroulis [413], pages 862–867. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000862000001&idtype=cvips.

Batzias:2007:MFD

[280] D. F. Batzias, V. Tsakiri, and D. K. Sidiras. A methodological framework for determining optimal dopant density in a biosensor transducer. In Simos and Maroulis [413],

pages 868–873. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000868000001&idtype=cvips`.

Reczynski:2007:CTE

[281] Witold Reczynski, Małgorzata Jakubowska, Bogusław Bas, Ewa Niewiara, and Władysław W. Kubiak. Chemometric tools in environmental data analysis. In Simos and Maroulis [413], pages 874–877. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000874000001&idtype=cvips`.

Batzias:2007:KBS

[282] A. F. Batzias, A. P. Efthymiadou, and C. G. Siontorou. A knowledge based system offering consultation for enhancing semi-natural wetland functionality. In Simos and Maroulis [413], pages 878–883. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000878000001&idtype=cvips`.

Fotilas:2007:SEI

[283] P. Fotilas and A. F. Batzias. Synthesizing equivalence indices for the comparative evaluation of technoeconomic efficiency of industrial processes at the design/re-engineering level. In Simos and Maroulis [413], pages 884–889. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000884000001&idtype=cvips`.

Mohammed:2007:RSH

[284] Avryl Mohammed, Kelvin Ramnath, Shyam Dyal, Francesca Lalla, and Jaipersad Roopchand. Rehabilitation of seven (7) hydrocarbon contaminated sites in a brackish water/lagoon environment in South Trinidad. In Simos and Maroulis [413], pages 890–893. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000890000001&idtype=cvips`.

Batzias:2007:DCC

[285] D. F. Batzias and Y. A. Pollalis. Determining capital cost in wastewater treatment installations operating under inflow characteristics uncertainty. In Simos and Maroulis [413], pages 894–899. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000894000001&idtype=cvips`.

Rode:2007:CML

[286] B. M. Rode and T. S. Hofer. Computational methods for the liquid state. In Simos and Maroulis [413], page 903. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000903000001&idtype=cvips`.

Marcos:2007:CMSb

[287] E. Sánchez Marcos, E. C. Beret, J. M. Martínez, R. R. Pappalardo, R. Ayala, and A. Muñoz-Páez. Coupling MD simulations and X-ray absorption spectroscopy to study ions in solution. In Simos and Maroulis [413], pages 904–908. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000904000001&idtype=cvips`.

Ayala:2007:API

[288] R. Ayala, J. M. Martinez, R. R. Pappalardo, A. Munoz-Paez, and E. Sanchez Marcos. The aquation of Po(IV): A quantum chemical study. In Simos and Maroulis [413],

pages 909–912. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000909000001&idtype=cvips`.

Rungrotmongkol:2007:UDT

[289] Thanyada Rungrotmongkol, Maturos Malaisree, Panita Decha, Chittima Laohpongspaisan, Ornjira Aruksakunwong, Pathumwadee Intharathep, Somsak Pianwanit, Pornthep Sompornpisut, Vudhichai Parasuk, Eugene Megnassan, Vladimir Frecer, Stanislav Miertus, and Supot Hannongbua. Understanding of drug-target interactions: A case study in influenza virus A subtype H5N1. In Simos and Maroulis [413], pages 913–916. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000913000001&idtype=cvips`.

Hofer:2007:CCS

[290] Thomas S. Hofer, Bernhard R. Randolf, and Bernd M. Rode. Computational challenges in simulation methods for liquids and solutions. In Simos and Maroulis [413], pages 917–920. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000917000001&idtype=cvips`.

Pribil:2007:SDC

[291] Andreas B. Pribil, Viwat Vchirawongkwin, Thomas S. Hofer, and Bernhard R. Randolf. Structure and dynamics of composite anions in aqueous solution. In Simos and Maroulis [413], pages 921–953. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000921000001&idtype=cvips`.

Xenides:2007:IQM

[292] Demetrios Xenides and Bernhard R. Randolf. Ab initio QM/MM simulations of water and hydrated cations. In Simos and Maroulis [413], pages 924–927. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000924000001&idtype=cvips`.

Tongraar:2007:PSD

[293] Anan Tongraar and Bernd M. Rode. Preferential solvation and dynamics of ions solvated in mixed solvents: Insights from QM/MM MD simulation approach. In Simos and Maroulis [413], pages 928–931. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000928000001&idtype=cvips`.

Caballero-Gil:2007:PSC

[294] Pino Caballero-Gil and Gerasimos C. Meletiou. Preface of the symposium 15: Cryptology, information security, and networks. In Simos and Maroulis [413], pages 935–936. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000935000001&idtype=cvips`.

Vasiliadis:2007:RPM

[295] D. C. Vasiliadis, G. E. Rizos, and C. Vassilakis. The role of priority mechanisms on performance metrics of double-buffered switching elements. In Simos and Maroulis [413], pages 937–942. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000937000001&idtype=cvips`.

Stergiou:2007:EMC

[296] E. Stergiou, G. Meletiou, D. C. Vasiliadis, G. E. Rizos, and S. V. Margariti. Evaluating the multicast control protocol on a multicasting network architecture. In Simos and

Maroulis [413], pages 943–946. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000943000001&idtype=cvips.

Rizos:2007:MWC

[297] G. E. Rizos and D. C. Vasiliadis. Multicasting in wireless communications (ad-hoc networks): Comparison against a tree-based approach. In Simos and Maroulis [413], pages 947–953. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000947000001&idtype=cvips.

Margariti:2007:SSC

[298] S. V. Margariti, G. Meletiou, E. Stergiou, D. C. Vasiliadis, and G. E. Rizos. Security systems consideration: A total security approach. In Simos and Maroulis [413], pages 954–958. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000954000001&idtype=cvips.

Tsiantis:2007:SIL

[299] L. E. Tsiantis, E. Stergiou, and S. V. Margariti. Security issues in E-learning systems. In Simos and Maroulis [413], pages 959–964. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000959000001&idtype=cvips.

Delgado:2007:SCD

[300] Oscar Delgado and Amparo Fúster. Stream cipher design for MANets. In Simos and Maroulis [413], pages 965–968. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000965000001&idtype=cvips.

Pazo-Robles:2007:MPS

[301] María Eugenia Pazo-Robles and Amparo Fúster-Sabater. Modeling pseudorandom sequence generators using cellular automata: The alternating step generator. In Simos and Maroulis [413], pages 969–972. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000969000001&idtype=cvips.

Mohatar:2007:NDO

[302] Oscar Delgado Mohatar and José M. Sierra Cámara. New directions in online fraud. In Simos and Maroulis [413], pages 973–976. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000973000001&idtype=cvips.

Li:2007:ISC

[303] Yiming Li. International Symposium on Computational Electronics — *Physical Modeling, Mathematical Theory, and Numerical Algorithms*. In Simos and Maroulis [413], page 979. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000979000001&idtype=cvips.

Jou:2007:SRN

[304] Yow-Jen Jou, Yung-Tsai Lu, Chien-Lun Lan, and Hsia Lee. Signal recognition by nonparametric discrimination of functional data for vehicle transportation system. In Simos and Maroulis [413], pages 980–983. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000980000001&idtype=cvips.

Jou:2007:SPL

[305] Yow-Jen Jou, Chai-Tzu Yang, Chien-Chia Huang, and Jennifer Yuh-Jen Wu. Semiparametric linear mixed effects model for vehicles identification. In Simos and Maroulis [413], pages 984–988. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000984000001&idtype=cvips.

Lo:2007:CDB

[306] Shih-Ching Lo. Classification of driving behavior by pattern recognition in multiclass users traffic flow. In Simos and Maroulis [413], pages 989–992. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000989000001&idtype=cvips.

Cho:2007:CST

[307] Hsun-Jung Cho and Heng Huang. A circuit simulation technique for congested network traffic assignment problem. In Simos and Maroulis [413], pages 993–996. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000993000001&idtype=cvips.

Li:2007:HFP

[308] Yiming Li and Ying-Chieh Chen. High frequency property optimization of heterojunction bipolar transistors using geometric programming. In Simos and Maroulis [413], pages 997–1000. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002000997000001&idtype=cvips.

Hwang:2007:NSN

[309] Chih-Hong Hwang and Yiming Li. Numerical simulation of nanoscale multiple-gate devices including random impurity effect. In Simos and Maroulis [413], pages 1001–1004. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001001000001&idtype=cvips.

Cho:2007:PPM

[310] Hsun-Jung Cho and Rih-Jin Li. A passing probability model for intelligent transportation system. In Simos and Maroulis [413], pages 1005–1008. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001005000001&idtype=cvips.

Li:2007:IST

[311] Yiming Li. International Symposium on Technology Management: Modeling, Simulation, and Optimization. In Simos and Maroulis [413], page 1011. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001011000001&idtype=cvips.

Wu:2007:EKF

[312] Wei-Wen Wu. Exploring KM features of high-performance companies. In Simos and Maroulis [413], pages 1012–1015. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001012000001&idtype=cvips.

Lo:2007:EAR

[313] Shih-Ching Lo and Yu Chao. Efficiency assessment of road project delivery models. In Simos and Maroulis [413], pages 1016–1019. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001016000001&idtype=cvips.

Cho:2007:PTNa

[314] Hsun-Jung Cho and Yi-Shan Li. On paradox of transportation networks. In Simos and Maroulis [413], pages 1020–1023. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001020000001&idtype=cvips`.

Cho:2007:HSP

[315] Hsun-Jung Cho and Chien-Lun Lan. A hybrid shortest path algorithm for navigation system. In Simos and Maroulis [413], pages 1024–1027. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001024000001&idtype=cvips`.

Cho:2007:PTNb

[316] Hsun-Jung Cho and Yi-Shan Li. On paradox of transportation networks. In Simos and Maroulis [413], pages 1028–1031. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001028000001&idtype=cvips`.

Cho:2007:MSB

[317] Hsun-Jung Cho and Guey-Shii Lin. Modeling and simulation of bus dispatching policy for timed transfers on signalized networks. In Simos and Maroulis [413], pages 1032–1035. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001032000001&idtype=cvips`.

Cho:2007:MSM

[318] Hsun-Jung Cho and Yuh-Ting Wu. Modeling and simulation of multiphase traffic flow. In Simos and Maroulis [413], pages 1036–1039. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001036000001&idtype=cvips`.

Li:2007:CSF

[319] Yiming Li, Yi-Hui Chiang, Shao-Ming Yu, Su-Yun Chiang, and C.-H. Hung. A comparative study of foreign direct investment flow using diffusion models. In Simos and Maroulis [413], pages 1040–1043. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001040000001&idtype=cvips`.

Lo:2007:EDB

[320] Shih-Ching Lo, Hsiao-Wei Tsai, Hsiao-Huei Wang, and Mong-Xi Chen. The effect of driving behavior on multiclass users traffic flow. In Simos and Maroulis [413], pages 1044–1047. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001044000001&idtype=cvips`.

Sakas:2007:SBM

[321] Damianos P. Sakas and Nikolaos Konstantopoulos. Symposium on business and management and dynamic simulation models supporting management strategies. In Simos and Maroulis [413], pages 1051–1053. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001051000001&idtype=cvips`.

Sakas:2007:CEB

[322] Damianos P. Sakas, Nikolaos Konstantopoulos, and Yiannis Triantafyllopoulos. Contribution of the executives in bank sector mergers: Application with a

simulation model. In Simos and Maroulis [413], pages 1054–1057. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001054000001&idtype=cvips.

Yiannis:2007:FAS

[323] Triantafyllopoulos Yiannis, Damianos P. Sakas, and Nikolaos Konstantopoulos. Factors that affect synergies in mergers, at banking sector: Simulation with a dynamic model. In Simos and Maroulis [413], pages 1058–1061. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001058000001&idtype=cvips.

Konstantopoulos:2007:DCM

[324] Nikolaos Konstantopoulos, Damianos P. Sakas, and Yiannis Triantafyllopoulos. The dimension of communication in the merger: Simulation with dynamic model. In Simos and Maroulis [413], pages 1062–1065. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001062000001&idtype=cvips.

Alexopoulos:2007:AGM

[325] A. B. Alexopoulos and Nikolaos Konstantopoulos. Analyzing the Greek marine manpower in the passenger and cruise markets using system dynamics. In Simos and Maroulis [413], pages 1066–1069. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001066000001&idtype=cvips.

Konstantopoulos:2007:CFS

[326] Nikolaos Konstantopoulos, Panagiotis Trivellas, and Panagiotis Reklitis. A conceptual framework of strategy, structure and innovative behaviour for the development of a dynamic simulation model. In Simos and Maroulis [413], pages 1070–1073. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001070000001&idtype=cvips.

Trivellas:2007:DSM

[327] Panagiotis Trivellas, Panagiotis Reklitis, and Nikolaos Konstantopoulos. A dynamic simulation model of organizational culture and business strategy effects on performance. In Simos and Maroulis [413], pages 1074–1077. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001074000001&idtype=cvips.

Stella:2007:ACA

[328] Michail G. Bekiaris Stella, A. Zounta, and Theodoros A. Stavrinoudis. Approaches to cost accounting in tourist management. In Simos and Maroulis [413], pages 1078–1081. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001078000001&idtype=cvips.

Kenourgios:2007:CGF

[329] Dimitris Kenourgios, Aristidis Samitas, and Nikolaos Konstantopoulos. The corporate governance framework and its application to privatizations of public enterprises. In Simos and Maroulis [413], pages 1082–1085. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001082000001&idtype=cvips.

Zondiros:2007:SMM

[330] Dimitris Zondiros, Nikolaos Konstantopoulos, and Petros Tomaras. A simulation model for measuring customer satisfaction through employee satisfaction. In Simos

and Maroulis [413], pages 1086–1089. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001086000001&idtype=cvips.

Konstantopoulos:2007:DSM

[331] Nikolaos Konstantopoulos, Michail G. Bekiaris, and Stella Zounta. A dynamic simulation model of the management accounting information systems (MAIS). In Simos and Maroulis [413], pages 1090–1093. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001090000001&idtype=cvips.

Reklitis:2007:OSB

[332] Panagiotis Reklitis, Nikolaos Konstantopoulos, and Panagiotis Trivellas. Organizational strategy and business environment effects based on a computation method. In Simos and Maroulis [413], pages 1094–1097. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001094000001&idtype=cvips.

Tomaras:2007:DPF

[333] Petros Tomaras, Nikolaos Konstantopoulos, and Dimitris Zondiros. The different paths in the franchising entrepreneurship choice. In Simos and Maroulis [413], pages 1098–1101. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001098000001&idtype=cvips.

Konstantopoulos:2007:HRM

[334] Nikolaos Konstantopoulos and Aristotelis B. Alexopoulos. The human resource management in dry-bulk shipping. In Simos and Maroulis [413], pages 1102–1105. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001102000001&idtype=cvips.

Konstantopoulos:2007:VSF

[335] Nikolaos Konstantopoulos, Petros Tomaras, and Dimitrios Zondiros. The values system in the franchising entrepreneurship. In Simos and Maroulis [413], pages 1106–1109. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001106000001&idtype=cvips.

Alexopoulos:2007:TQM

[336] Aristotelis B. Alexopoulos and Nikolaos Konstantopoulos. Total quality management in dry-bulk shipping. In Simos and Maroulis [413], pages 1110–1113. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001110000001&idtype=cvips.

Abietar:2007:DST

[337] José M. Abietar, Pedro J. Morcillo, and Ginés Moreno. Designing a software tool for fuzzy logic programming. In Simos and Maroulis [413], pages 1117–1120. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001117000001&idtype=cvips.

Abramczyk:2007:FDB

[338] H. Abramczyk, I. Placek, uska, K. Kurczewski, Z. Morawiec, and M. Tazbir. From femtosecond dynamics to breast cancer diagnosis by Raman spectroscopy. In Simos and Maroulis [413], pages 1121–1124. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001121000001&idtype=cvips.

Abu-Dawwas:2007:PDP

[339] Waheeb A. Abu-Dawwas, Rashed M. Al-Azzeh, and Mohammed H. Abu-Arqoub. Psycho-diagnostic problems of personalized teaching systems. In Simos and Maroulis [413], pages 1125–1127. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001125000001&idtype=cvips.

Abudu:2007:RNE

[340] Bolanle Abudu and Sheri Markose. Relational neural evolution approach to bank failure prediction. In Simos and Maroulis [413], pages 1128–1131. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001128000001&idtype=cvips.

Akhmetov:2007:ALM

[341] Dauren F. Akhmetov and Minoru Kotaki. Aggregative learning method and its application for communication quality evaluation. In Simos and Maroulis [413], pages 1132–1135. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001132000001&idtype=cvips.

Alarcon:2007:UIG

[342] Vladimir J. Alarcon, Charles G. O'Hara, Roland Viger, Bijay Shrestha, and Preeti Mali. Using an interoperable geoprocessing system for hydrological simulation. In Simos and Maroulis [413], pages 1136–1140. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001136000001&idtype=cvips.

Alberto:2007:NSS

[343] A. Alberto, E. Arias, T. Rojo, F. Cuartero, and J. Benet. Numerical simulation of the static stiffness problem on a catenary by using threads. In Simos and Maroulis [413], pages 1141–1145. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001141000001&idtype=cvips.

Balsas:2007:KPR

[344] M. C. Balsas, E. S. Jiménez, and J. A. Vera. The Kepler problem in rotating reference frames: Topological study of the phase flow. In Simos and Maroulis [413], pages 1146–1149. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001146000001&idtype=cvips.

Barabas:2007:TAE

[345] Béla Barabás, Luciano Caglioti, Francesco Faglioni, Nicola Florini, Paolo Lazzeretti, Marco Maioli, Gyula Rábai, Ferdinando Taddei, Claudia Zucchi, and Gyula Pályi. On the traces of absolute enantioselective synthesis. In Simos and Maroulis [413], pages 1150–1152. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001150000001&idtype=cvips.

Bayon:2007:CCD

[346] L. Bayón, J. M. Grau, M. M. Ruiz, and P. M. Suárez. The cyclic coordinate descent in hydrothermal optimization problems with non-regular Lagrangian. In Simos and Maroulis [413], pages 1153–1157. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001153000001&idtype=cvips.

Bougouffa:2007:NTS

[347] Smail Bougouffa and Saud Al-Awfi. Numerical treatment of Schrödinger coupled differential equations. In Simos and Maroulis [413], pages 1158–1161. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001158000001&idtype=cvips.

Bozejko:2007:AMM

[348] W. Bozejko and M. Wodecki. Applying multi-moves in parallel genetic algorithm for the flow shop problem. In Simos and Maroulis [413], pages 1162–1165. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001162000001&idtype=cvips.

Cambrini:2007:WSD

[349] Luigi Cambrini, Jürgen Biber, Dieter Hönigmann, and Maike Löhndorf. Weld spot detection by color segmentation and template convolution. In Simos and Maroulis [413], pages 1166–1169. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001166000001&idtype=cvips.

Chin:2007:RDS

[350] Pius W. M. Chin, Jean M.-S. Lubuma, and Kailash C. Patidar. Regularity and discrete schemes for the heat equation on non-smooth domains. In Simos and Maroulis [413], pages 1170–1173. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001170000001&idtype=cvips.

Czernek:2007:USC

[351] Jirí Czernek. The UCCSD(T)/CBS description of the C_{2h} symmetric, negatively charged dimer of SF_2. In Simos and Maroulis [413], pages 1174–1177. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001174000001&idtype=cvips.

Nori-Shargh:2007:SDB

[352] Davood Nori-Shargh and Fahimeh Roohi. Structures and dynamic behaviors of tetrahydridodimetallenes, M2H4, (M = Si, Ge, Sn): A DFT study and NBO analysis. In Simos and Maroulis [413], pages 1178–1182. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001178000001&idtype=cvips.

Demiralp:2007:EMB

[353] Metin Demıralp. Expectation matrix based quantum dynamics of a univariate system at the zero fluctuation limit. In Simos and Maroulis [413], pages 1183–1186. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001183000001&idtype=cvips.

Gkritzapis:2007:SDF

[354] Dimitrios N. Gkritzapis, Elias E. Panagiotopoulos, Dionissios P. Margaris, and Dimitrios G. Papanikas. A six degree of freedom trajectory analysis of spin-stabilized projectiles. In Simos and Maroulis [413], pages 1187–1194. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001187000001&idtype=cvips.

Domingues:2007:SPHb

[355] Guilherme Domingues, Yoshiyuki Morie, Feng Long Gu, Takeshi Nanri, and Kazuaki Murakami. SMMH — A parallel heuristic for combinatorial opti-

mization problems. In Simos and Maroulis [413], pages 1195–1198. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001195000001&idtype=cvips.

Ferrero:2007:CPH

[356] M. Ferrero, Michel Rérat, R. Orlando, and R. Dovesi. Coupled perturbed Hartree–Fock calculation of the static polarizability for periodic systems: Implementation in the CRYSTAL code. In Simos and Maroulis [413], pages 1199–1203. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001199000001&idtype=cvips.

Ghadarghadr:2007:MCS

[357] Y. Ghadarghadr and S. M. Hashemianzadeh. Monte Carlo simulation of the adsorption of methane and tetrafluorocarbon on single walled carbon nanotubes. In Simos and Maroulis [413], pages 1204–1207. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001204000001&idtype=cvips.

Gille:2007:RDD

[358] Wilfried Gille. Reconstruction of a destroyed 'dead leaves' tessellation from its fragments via the puzzle fitting function. In Simos and Maroulis [413], pages 1208–1211. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001208000001&idtype=cvips.

Gunay:2007:TPU

[359] Seçkin D. Gunay, Unsal Akdere, Birtan Kavanoz, and Çetin Ta. Transport properties of uranium dioxide by molecular dynamics simulation. In Simos and Maroulis [413], pages 1212–1215. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001212000001&idtype=cvips.

Hayes:2007:IES

[360] Jer Hayes, John Cleary, Conor Slater, King Tong Lau, and Dermot Diamond. Intelligent environmental sensing with a phosphate monitoring system and online resources. In Simos and Maroulis [413], pages 1216–1219. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001216000001&idtype=cvips.

Hernandez:2007:VAF

[361] Gonzalo Hernández, Cesar Fernández, Roberto León, and Luís Salinas. Visualizations of a n-ary fragmentation process with neighborhood interaction. In Simos and Maroulis [413], pages 1220–1223. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001220000001&idtype=cvips.

Hosokawa:2007:IEE

[362] Kiyotada Hosokawa and Shin ichiro Sato. Interpretation of electronically excited states by means of configuration analysis. In Simos and Maroulis [413], pages 1224–1227. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001224000001&idtype=cvips.

Hsu:2007:TIS

[363] Nai-Wen Hsu, Jr-Shiuan Liang, and Yi-Chang Chen. Taiwan's information security policy enhancement: an analysis of patent indicators and patent documents. In Simos

and Maroulis [413], pages 1228–1231. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001228000001&idtype=cvips.

Iliadis:2007:ANN

[364] L. S. Iliadis and S. I. Spartalis. Artificial neural networks equivalent to fuzzy algebra T-norm conjunction operators. In Simos and Maroulis [413], pages 1232–1235. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001232000001&idtype=cvips.

Jabbarzadeh:2007:MDS

[365] A. Jabbarzadeh and R. I. Tanner. Molecular dynamics simulation of crystallization under quiescent and shearing conditions. In Simos and Maroulis [413], pages 1236–1239. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001236000001&idtype=cvips.

Jelinek:2007:MRD

[366] P. Jelínek, P. Virostko, Z. Hubicka, and P. Bartos. Modelling of RF discharge in argon plasma. In Simos and Maroulis [413], pages 1240–1243. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001240000001&idtype=cvips.

Kabelac:2007:NMD

[367] Martin Kabelác, Haydee Valdes, Edward C. Sherer, Christopher J. Cramer, and Pavel Hobza. New MP2 database of nucleic acid base trimers: How well reproduce DFT methods structure and binding energies? In Simos and Maroulis [413], pages 1244–1247. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001244000001&idtype=cvips.

Kabongo:2007:STP

[368] Luis Kabongo, Pascal Desbarats, and Erik Dumont. A step towards planification of focused ultrasound thermoablation. In Simos and Maroulis [413], pages 1248–1252. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001248000001&idtype=cvips.

Kalogiratou:2007:EFP

[369] Z. Kalogiratou, Th. Monovasilis, and T. E. Simos. An exponentially fitted 6(4) pair of explicit Runge–Kutta–Nyström methods. In Simos and Maroulis [413], pages 1253–1256. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001253000001&idtype=cvips.

Kazerooni:2007:STF

[370] Reza Bahoosh Kazerooni and Siamak Kazemzadeh Hannani. Simulation of turbulent flow through porous media employing a v2f model. In Simos and Maroulis [413], pages 1257–1260. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001257000001&idtype=cvips.

Komeiji:2007:IFM

[371] Yuto Komeiji, Takeshi Ishikawa, Yuji Mochizuki, Hiroshi Yamataka, and Tatsuya Nakano. *Ab initio* FMO–MD method reimplemented and applied to pure water. In Simos and Maroulis [413], pages 1261–1264. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001261000001&idtype=cvips.

Lohndorf:2007:OVQ

[372] Maike Löhndorf, Herbert Ramoser, and Luigi Cambrini. Online visual quality inspection for weld seams. In Simos and Maroulis [413], pages 1265–1268. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001265000001&idtype=cvips.

Loukopoulos:2007:NSV

[373] V. C. Loukopoulos and G. T. Karahalios. Numerical solution of the velocity–vorticity Navier–Stokes equations in three dimensions for an incompressible Newtonian fluid. In Simos and Maroulis [413], pages 1269–1272. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001269000001&idtype=cvips.

Lu:2007:PHT

[374] Jun Lu and Liaofu Luo. Predicting human transcription starts by use of diversity measure with quadratic discriminant. In Simos and Maroulis [413], pages 1273–1277. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001273000001&idtype=cvips.

Luo:2007:SPR

[375] Liaofu Luo and Jun Lu. Sequence pattern recognition in genome analysis. In Simos and Maroulis [413], pages 1278–1281. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001278000001&idtype=cvips.

Makowski:2007:PMF

[376] Mariusz Makowski and Lech Chmurzyński. Potentials of mean force of two hydrophobic amino-acid side chain models dependent on orientation. In Simos and Maroulis [413], pages 1282–1284. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001282000001&idtype=cvips.

Matias:2007:AEI

[377] J. M. Matías, T. Rivas, C. Ordóñez, and J. Taboada. Assessing the environmental impact of slate quarrying using Bayesian networks and GIS. In Simos and Maroulis [413], pages 1285–1288. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001285000001&idtype=cvips.

Matias:2007:FEP

[378] J. M. Matías, L. Bayón, P. Suárez, A. Argüelles, and J. Taboada. Forecasting electricity prices in an optimization hydrothermal problem. In Simos and Maroulis [413], pages 1289–1292. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001289000001&idtype=cvips.

Lain:2007:ITO

[379] Mohamed Ras Lain and Abdelhafid Chaabi. Influence of temperature on the offset voltage of piezoresistive pressure sensors. In Simos and Maroulis [413], pages 1293–1297. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001293000001&idtype=cvips.

Mahmood:2007:CGC

[380] Mohammed Shuker Mahmood. A conservative Galerkin-characteristics algorithm combined with a relaxation scheme for two regions nonlinear solute transport problem in porous media. In Simos and Maroulis [413], pages 1298–1301. .

URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001298000001&idtype=cvips.

Monaco:2007:ASO

[381] Guglielmo Monaco and Riccardo Zanasi. Analysis of some orbital contributions to the current density in circulenes. In Simos and Maroulis [413], pages 1302–1305. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001302000001&idtype=cvips.

Monovasilis:2007:FTF

[382] Th. Monovasilis, Z. Kalogiratou, and T. E. Simos. A family of trigonometrically-fitted partitioned Runge–Kutta symplectic methods. In Simos and Maroulis [413], pages 1306–1310. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001306000001&idtype=cvips.

Nateghi:2007:TSD

[383] Mohammad R. Nateghi and F. Kalantari. Theoretical study of 1,8-diaminonaphthalene polymerization. In Simos and Maroulis [413], pages 1311–1314. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001311000001&idtype=cvips.

Niakas:2007:AFD

[384] N. Niakas, V. C. Loukopoulos, and C. Douskos. An accurate finite-difference scheme on second order partial differential equations in 3D. In Simos and Maroulis [413], pages 1315–1318. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001315000001&idtype=cvips.

Nieto:2007:AAS

[385] P. J. García Nieto, J. J. del Coz Díaz, J. A. Vilán Vilán, and F. P. Alvarez Rabanal. Acoustic analysis of a sandwich non metallic panel for roofs by FEM and experimental validation. In Simos and Maroulis [413], pages 1319–1322. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001319000001&idtype=cvips.

Papadopoulos:2007:ACM

[386] Polycarpos K. Papadopoulos and Pavlos M. Hatzikonstantinou. Application of the CVP method on 3D internal flows. In Simos and Maroulis [413], pages 1323–1326. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001323000001&idtype=cvips.

Papakonstantinou:2007:ENV

[387] K. Papakonstantinou, C. Belias, N. Vlachakis, and I. Statharas. Evaluation of a natural ventilation configuration at a public building. In Simos and Maroulis [413], pages 1327–1330. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001327000001&idtype=cvips.

Pedesseau:2007:ACA

[388] L. Pedesseau, J. Even, F. Doré, and C. Cornet. Atomic calculations applied to semiconductor hetero structures. In Simos and Maroulis [413], pages 1331–1334. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001331000001&idtype=cvips.

Petrovic-Lazarevic:2007:UNF

[389] Sonja Petrovic-Lazarevic and Jian Ying Zhang. Usefulness of neuro-fuzzy models' application for tobacco control. In Simos and Maroulis [413], pages 1335–1338.

. URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001335000001&idtype=cvips`.

Pluhackova:2007:TIU

[390] Kristýna Pluhácková and Pavel Hobza. Theoretical investigation of the unexpected red shift in the halothane ··· acetone complex. In Simos and Maroulis [413], pages 1339–1342. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001339000001&idtype=cvips`.

Romaguera:2007:CMC

[391] S. Romaguera, M. P. Schellekens, P. Tirado, and O. Valero. Contraction maps on complexity spaces and itExpoDC algorithms. In Simos and Maroulis [413], pages 1343–1346. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001343000001&idtype=cvips`.

Ruiz:2007:JLC

[392] Irene Luque Ruiz and Miguel Ángel Gómez-Nieto. A Java library for the calculation of molecular descriptors. In Simos and Maroulis [413], pages 1347–1350. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001347000001&idtype=cvips`.

Sakas:2007:FCB

[393] D. P. Sakas, D. S. Vlachos, and T. E. Simos. Fuzzy constraint based model for efficient management of dynamic purchasing environments. In Simos and Maroulis [413], pages 1351–1354. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001351000001&idtype=cvips`.

Sakas:2007:ANN

[394] D. P. Sakas, D. S. Vlachos, and T. E. Simos. Adaptive neural networks for automatic negotiation. In Simos and Maroulis [413], pages 1355–1358. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001355000001&idtype=cvips`.

Sakas:2007:ATO

[395] D. P. Sakas, D. S. Vlachos, and T. E. Simos. Adaptive techniques for online auctions. In Simos and Maroulis [413], pages 1359–1362. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001359000001&idtype=cvips`.

Savchenko:2007:CEC

[396] Nicolai D. Savchenko, Tatiana N. Shchurova, Alexander B. Kondrat, and Vladimir M. Mitsa. Calculation of elastic constants for $(GeS_2)_x$ $(As_2\ S_3)_{1-x}$ glasses. In Simos and Maroulis [413], pages 1363–1366. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001363000001&idtype=cvips`.

Shao:2007:NSF

[397] J. Shao and C. Zhang. Numerical studies of flow past two side-by-side circular cylinders. In Simos and Maroulis [413], pages 1367–1370. . URL `http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001367000001&idtype=cvips`.

Shigeta:2007:QCD

[398] Yasuteru Shigeta. Quantal cumulant dynamics for dissipative systems. In Simos and Maroulis [413], pages 1371–1374. . URL `http://proceedings.aip.org/getpdf/`

servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001371000001&idtype=cvips.

Soares:2007:TSO

[399] T. A. Soares and T. P. Straatsma. Towards simulations of outer membrane proteins in lipopolysaccharide membranes. In Simos and Maroulis [413], pages 1375–1378. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001375000001&idtype=cvips.

Straatsma:2007:DIA

[400] T. P. Straatsma. Data intensive analysis of biomolecular simulations. In Simos and Maroulis [413], pages 1379–1382. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001379000001&idtype=cvips.

Tsakstara:2007:CMN

[401] V. Tsakstara, T. S. Kosmas, J. Sinatkas, V. C. Chasioti, and P. C. Divari. The convolution method in neutrino physics searches. In Simos and Maroulis [413], pages 1383–1387. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001383000001&idtype=cvips.

Utkin:2007:MDS

[402] A. V. Utkin, I. F. Golovnev, and V. M. Fomin. Molecular dynamic simulation of detonation phenomena. In Simos and Maroulis [413], pages 1388–1391. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001388000001&idtype=cvips.

Vlachos:2007:IRT

[403] D. S. Vlachos and C. G. Tsabaris. Image recognition techniques for gamma spectroscopy. In Simos and Maroulis [413], pages 1392–1395. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001392000001&idtype=cvips.

Vlachos:2007:ODK

[404] D. S. Vlachos, O. T. Kosmas, and T. E. Simos. Optimized derivative kernels for gamma ray spectroscopy. In Simos and Maroulis [413], pages 1396–1399. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001396000001&idtype=cvips.

Voracek:2007:IDS

[405] Michal Vorácek, Ladislav Vagner, and Tomás Flouri. Indexing degenerate strings. In Simos and Maroulis [413], pages 1400–1403. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001400000001&idtype=cvips.

Vural:2007:IND

[406] Cabir Vural and Serap Kazan. Image normalization and discrete wavelet transform based robust digital image watermarking. In Simos and Maroulis [413], pages 1404–1407. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001404000001&idtype=cvips.

Xenides:2007:FNC

[407] D. Xenides, D. S. Vlachos, and T. E. Simos. Fuzzy neural classifiers for multi-wavelength interdigital sensors. In Simos and Maroulis [413], pages 1408–1411.

. URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001408000001&idtype=cvips.

Yin:2007:NHA

[408] Aihua Yin and Shousheng Zhang. A new heuristic algorithm for solving the job shop scheduling problem. In Simos and Maroulis [413], pages 1412–1416. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001412000001&idtype=cvips.

Zhang:2007:NME

[409] L. Zhang, C. Zhang, and R. Martinuzzi. Numerical modeling of energy consumption in a typical residential building. In Simos and Maroulis [413], pages 1417–1420. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001417000001&idtype=cvips.

Zurek:2007:DIB

[410] Eva Zurek, Jochen Autschbach, and Ole Krogh Andersen. Downfolding and N-ization of basis sets of Slater Type Orbitals. In Simos and Maroulis [413], pages 1421–1424. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001421000001&idtype=cvips.

Zurek:2007:DFS

[411] Eva Zurek and Jochen Autschbach. Density functional studies of the ^{13}C NMR chemical shifts in single-walled carbon nanotubes. In Simos and Maroulis [413], pages 1425–1428. . URL http://proceedings.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=APCPCS000963000002001425000001&idtype=cvips.

Maroulis:2007:CMS

[412] George Maroulis and Theodore E. Simos, editors. *Computational Methods in Science and Engineering: Theory and Computation: Old Problems and New Challenges. Lectures Presented at the International Conference on Computational Methods in Science and Engineering 2007 (ICCMSE 2007): Corfu (Greece), 25–30 September 2007*, volume 1 of *AIP Conference Proceedings (#963)*. American Institute of Physics, Woodbury, NY, USA, 2007. URL http://www.springer.com/physics/atoms/book/978-0-7354-0477-9.

Simos:2007:CMS

[413] Theodore E. Simos and George Maroulis, editors. *Computation in Modern Science and Engineering: Proceedings of the [Fifth] International Conference on Computational Methods in Science and Engineering 2007 (ICCMSE 2007), Corfu, Greece, 25–30 September 2007*, volume 2A, 2B of *AIP Conference Proceedings (#963)*. American Institute of Physics, Woodbury, NY, USA, 2007. . URL http://www.springer.com/physics/atoms/book/978-0-7354-0478-6.