

IUPAP C20 Conference on Computational Physics

(CCP 2011)

Journal of Physics: Conference Series Volume 402

**Gatlinburg, Tennessee, USA
16-20 October 2011**

Editors:

**G Malcolm Stocks
M Claudia Troparevsky**

**ISBN: 978-1-62276-868-4
ISSN: 1742-6588**

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2011) by the Institute of Physics
All rights reserved.

Printed by Curran Associates, Inc. (2013)

For permission requests, please contact the Institute of Physics
at the address below.

Institute of Physics
Dirac House, Temple Back
Bristol BS1 6BE UK

Phone: 44 1 17 929 7481
Fax: 44 1 17 920 0979

techtracking@iop.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

Materials/condensed matter theory and nano science

012001 [Temperature dependence in interatomic potentials and an improved potential for Ti](#) G J Ackland 1

012002 [Simulations of nanosensors based on single walled carbon nanotubes](#) Polina Pine, Yuval E Yaish and Joan Adler 10

012003 [Monte Carlo Simulation of Secondary Electron Emission from Dielectric Targets](#) Maurizio Dapor 16

012004 [Electronic properties of rippled graphene](#) Gui Gu, Jianxin Zhong and Zhenqiang Ma 27

012005 [Structural search for dense packing of concave and convex shapes in two dimensions](#) Nabiha T Elias and Toby S Hudson 32

012006 [Investigating robustness of interatomic potentials with universal interface](#) Bohumir Jelinek, Kiran Solanki, John F Peters and Sergio D Felicelli 39

012007 [Symbolic programming package N_Coperators with applications to theoretical atomic spectroscopy](#) Rytis Juršėnas and Gintaras Merklelis 44

012008 [Hybrid algorithms in quantum Monte Carlo](#) Jeongnim Kim, Kenneth P Esler, Jeremy McMinis, Miguel A Morales, Bryan K Clark, Luke Shulenburger and David M Ceperley 54

012009 [Dynamics of chemical reacting systems in low dimensional lattices via the Equation Free Method](#) Giacomo Mazzi 66

012010 [The use of atomic level stress to characterize the structure of irradiated iron](#) Madhusudan Ojha, D M Nicholson, Kh Odbadrakh, Bala Radhakrishnan, R E Stoller and Takeshi Egami 72

012011 [Coarse Grained Approach to First Principles Modeling of Radiation Cascade in Large Fe Supercells](#) Kh Odbadrakh, D M Nicholson, A Rusanu, G D Samolyuk, R E Stoller, X-G Zhang and G M Stocks 78

012012 [Ab initio molecular dynamics study of diffusion mechanism in liquid B₂O₃ under pressure](#) Satoshi Ohmura and Fuyuki Shimojo 85

012014 [Irreversible Thermodynamics](#) David M Rogers and Susan B Rempe 92

012015 [Efficient non-equidistant FFT approach to the measurement of single- and two-particle quantities in continuous time Quantum Monte Carlo methods](#) Peter Staar, Thomas A Maier and Thomas C Schultheiss 108

012016 [Electron Transfer on Impurity doped Graphene Nanoribbon](#) Hiroyoshi Tsuyuki, Shoichi Sakamoto and Mitsuyoshi Tomiya 121

Strongly correlated systems and quantum phase transitions

012017 [The Universal Edge Physics in Fractional Quantum Hall Liquids](#) Zi-Xiang Hu, R N Bhatt, Xin Wan and Kun Yang 124

012018 [Numerical linked-cluster expansion for the distorted kagome lattice Heisenberg model](#) Ehsan Khatami and Marcos Rigol 131

012019 [An Efficient Algorithm for Simulating the Real-Time Quantum Dynamics of a Single Spin-1/2 Coupled to Specific Spin-1/2 Baths](#) M A Novotny, M Guerra, H De Raedt, K Michielsen and F Jin 138

012020 [Numerical studies of the fractional quantum Hall effect in systems with tunable interactions](#) Z Papić, D A Abanin, Y Barlas and R N Bhatt 155

012021 [The fractional quantum Hall effect at filling factor 5/2: numerically searching for non-abelian anyons](#) Michael R Peterson 164

012022 [Spin waves in the classical Heisenberg antiferromagnet on the kagome lattice](#) Stefan Schnabel and David P Landau 178

Astrophysics

012023 [On Simulating Type Ia Supernovae](#) A C Calder, B K Krueger, A P Jackson, D M Townsley, E F Brown and F X Timmes 187

012024 [Conservative Initial Mapping For Multidimensional Simulations of Stellar Explosions](#) Ke-Jung Chen, Alexander Heger and Ann Almgren 200

012025 [Advancements in modeling self-consistent core collapse supernovae with CHIMERA](#) M A Chertkow, O E B Messer, W R Hix, C T Lee, K Yakunin, P Marronetti, S W Bruenn, E J Lentz, J Blondin and A Mezzacappa 207

012026 [Phase diagram of carbon-oxygen plasma mixtures in white dwarf stars](#) A S Schneider, C J Horowitz, J Hughto and D K Berry 218

012027 [Turbulent magnetic field amplification from spiral SASI modes in core-collapse supernovae](#) E Endeve, C Y Cardall, R D Budiardja and A Mezzacappa 232

012028 [Ash-detonation interactions in multi-dimensional simulation of Type Ia supernovae](#) S T Parete-Koon, C R Smith, M W Guidry, W R Hix and O E B Messer 247

Nuclear and high energy physics

012029 [Parallel computation of Feynman loop integrals](#) E de Doncker and F Yuas 254

012030 [Microscopic nuclear mass table with high-performance computing](#) J Erler, N Birge, M Kortelainen, W Nazarewicz, E Olsen, A Perhac and M Stoitsov 262

012031 [Ab Initio Nuclear Structure Calculations of Light Nuclei](#) Pieter Maris 269

012032 [Real-time calculations of many-body dynamics in quantum systems](#) Takashi Nakatsukasa 283

012033 [*UNEDF: Advanced Scientific Computing Collaboration Transforms the Low-Energy Nuclear Many-Body Problem*](#) H Nam, M Stoitsov, W Nazarewicz, A Bulgac, G Hagen, M Kortelainen, P Maris, J C Pei, K J Roche, N Schunck, I Thompson, J P Vary and S M Wild 298

012034 [Reflection-asymmetric nuclear deformations within the Density Functional Theory](#) E Olsen, J Erler, W Nazarewicz and M Stoitsov 310

012035 [Coordinate-Space Hartree-Fock-Bogoliubov Solvers for Super fluid Fermi Systems in Large Boxes](#) J C Pei, G I Fann, R J Harrison, W Nazarewicz, J Hill, D Galindo and J Jia 317

012036 [Numerical study of hot strongly interacting matter](#) P Petreczky 324

012037 [From nucleons to nuclei to fusion reactions](#) S Quaglioni, P Navrátil, R Roth and W Horiuchi 339

012038 [Microscopic calculation of heavy-ion potentials based on TDHF](#) A S Umar and V E Oberacker 356

Macroscopic transport, mesoscopic methods and related

012039 [A model for stable interfacial crack growth](#) Knut S Gjerden, Arne Stormo and Alex Hansen 371

012040 [Preconditioner methods applied to simulations of two-phase flow in porous media](#) Morten Grøva 379

012041 [Statistical Law of Turbulence in Granular Gas](#) Masaharu Isobe 388

012042 [Morphology diagrams for \$A_2B\$ copolymer melts: real-space self-consistent field theory](#) Rajeev Kumar, Yige Li, Scott W Sides, Jimmy W Mays and Bobby G Sumpter 396

012043 [Comparison of Phase Field Crystal and Molecular Dynamics Simulations for a Shrinking Grain](#) B Radhakrishnan, S B Gorti, D M Nicholson and J Dantzig 403

012044 [Molecular-Dynamics Study of Void-Formation inside Silicon Wafers in Stealth Dicing](#) K Shimamura, J Okuma, S Ohmura and F Shimojo 410

012045 [Influence of Heat Source Characteristics on Dimensionless Thermal Spreading Resistance](#) A L Wang and C P Yan 419

Biological physics

012046 [Surface adsorption of lattice HP proteins: Thermodynamics and structural transitions using Wang-Landau sampling](#) Ying Wai Li, Thomas Wüst and David P Landau 430

012047 [Driving Calmodulin Protein towards Conformational Shift by Changing Ionization States of Select Residues](#) Sunita Negi, Ali Rana Atilgan and Canan Atilgan 437

012048 [Conformational transitions of a confined lattice protein: A Wang-Landau study](#) Busara Pattanasiri, Ying Wai Li, David P Landau, Thomas Wüst and Wannapong Triampo 447