30th Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics 2017

Journal of Physics: Conference Series Volume 921

Athens, Georgia, USA
20 – 24 February 2017

ISBN: 978-1-5108-5341-6
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.

Printed by Curran Associates, Inc. (2018)

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: 845-758-2633
Email: curran@proceedings.com
Web: www.proceedings.com

Table of contents

Volume 921

30th Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics

20–24 February 2017, University of Georgia, USA

Accepted papers received: 30 October 2017
Published online: 19 November 2017

Preface

30th Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics

Peer review statement

Papers

An open-source job management framework for parameter-space exploration: OACIS

Y. Murase, T. Uchitane and N. Ito.....1

Interactions between proteins and poly(ethylene-glycol) investigated using molecular dynamics simulations

Giovanni Settanni, Jiajia Zhou and Friederike Schmid.....10

Universality and phase diagrams of the Baxter-Wu Model in a Crystal Field: spin-1 and spin-3/2

D. A. Dias, J. C. Xavier and J. A. Plascak.....17

The zeros of the Energy Probability Distribution - A new way to study phase transitions -

B. V. Costa, L. A. S. Mól and J. C. S. Rocha.....21

Applying Renormalization Group to Quantum Walks

S. Boettcher.....28

Collective motion in repulsive self-propelled particles in confined geometries

Takayuki Hiraoka, Takashi Shimada and Nobuyasu Ito.....32

Combined molecular and spin dynamics simulation of bcc iron with lattice vacancies

Mark Mudrick, Markus Eisenbach, Dilina Perera, G. Malcolm Stocks and David P. Landau.....37

A study of vibrating nanotubes with additional adsorbed masses

Joan Adler and Omri Adler.....42

Accuracy and Transferability of *Ab Initio* Electronic Band Structure Calculations for Doped $BiFeO_3$

Julian Gebhardt and Andrew M. Rappe.....48

Structure of transition metal clusters: A force-biased Monte Carlo approach

Dil K. Limbu and Parthapratim Biswas.....58

An iterative aggregation and disaggregation approach to the calculation of steady state distributions of continuous processes

Katja Biswas.....63

[High resolution Monte Carlo study of the Domb-Joyce model]

Nathan Clisby.....73

[Application of artificial neural networks to identify equilibration in computer simulations]

Mitchell H Leibowitz, Evan D Miller, Michael M Henry and Eric Jankowski.....78

[Interface of topological insulator Bi_2Se_3 with As_2Te_3]

Niraj Aryal and Efstratios Manousakis.....86

[Shape matters: The case for Ellipsoids and Ellipsoidal Water*]

Andreas F. Tillack and Bruce H. Robinson.....90

[Yaldram-Khan model with CO and N desorption]

Jonás Díaz and Gloria María Buendía.....95

[Population annealing: Massively parallel simulations in statistical physics]

Martin Weigel, Lev Yu. Barash, Michal Borovský, Wolfhard Janke and Lev N. Shchur.....100

[Transition barrier at a first-order phase transition in the canonical and microcanonical ensemble]

Wolfhard Janke, Philipp Schierz and Johannes Zierenberg.....110

[Density of states for systems with multiple order parameters: a constrained Wang-Landau method]

Chor-Hoi Chan, Gregory Brown and Per Arne Rikvold.....115