

26th Annual CSP Workshop on Recent Developments in Computer Simulation Studies in Condensed Matter Physics

(CSP 2013)

Physics Procedia Volume 53

**Athens, Georgia, USA
25 February – 1 March 2013**

ISBN: 978-1-63266-911-7

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© by Elsevier B.V.
All rights reserved.

Printed by Curran Associates, Inc. (2014)

For permission requests, please contact Elsevier B.V.
at the address below.

Elsevier B.V.
Radarweg 29
Amsterdam 1043 NX
The Netherlands

Phone: +31 20 485 3911
Fax: +31 20 485 2457

<http://www.elsevierpublishingsolutions.com/contact.asp>

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



ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Physics Procedia 53 (2014) iii

Physics

Procedia

Preface	1
D.P. Landau, M. Bachmann, S.P. Lewis, H.-B. Schüttler	1
Educating the Next Generation of Computational Physicists	
J. Adler	2
Density and Diffusion Anomalies in a Repulsive Lattice Gas	
A.A. Bertolazzo, M.C. Barbosa	7
Pattern-recognising Polymer Adsorption on Structured Surfaces: Gaussian Polymers vs. Freely Jointed Chains	
H. Behringer	16
Extremal Optimization for Ground States of the Sherrington-Kirkpatrick Spin Glass with Levy Bonds	
S. Boettcher	24
Convergence in Flat-Histogram Sampling	
G. Brown	28
Integrated Experimental and Computational Studies of Energy-relevant Interfaces	
G. Feng, P.T. Cummings	32
FIT-MART: Quantum Magnetism with a Gentle Learning Curve	
L. Engelhardt, S.C. Garland, C. Rainey, R.A. Freeman	39
The Use of Monte Carlo Simulation to Obtain the Wetting Properties of Water	
V. Kumar, J.R. Errington	44
Statistical Analysis of the Influence of Interaction Ranges on Structural Phases of Flexible Polymers	
J. Gross, T. Neuhaus, T. Vogel, M. Bachmann	50
Scaling Properties of Parallelized Multicanonical Simulations	
J. Zierenberg, M. Marenz, W. Janke	55
Issues on the Choice of a Proper Time Step in Molecular Dynamics	
S. Kim	60
Determining Bulk Equilibrium Constants for Cluster Formation from Constant <i>NVT</i> Ensemble Simulations at Small <i>N</i>	
J.T. Kindt	63
Quantum Transport through a Fully Connected Network with Disorder	
M.A. Novotny, L. Solomon, G. Inkoorn	71
Molecular Dynamics Models of Shaped Particles Using Filling Solutions	
C.L. Phillips, J.A. Anderson, S.C. Glotzer	75
Phase Separation on a Hyperbolic Lattice	
J. Raffield, H.L. Richards, J. Molchanoff, P.A. Rikvold	82
Thermodynamics of Protein Aggregation	
K.L. Osborne, B. Barz, M. Bachmann, B. Strodel	90
Fourier Monte Carlo Implementation Guide	
A. Tröster	96