## Contents

A Discontinuous Potential Model for Protein–Protein Interactions .......................... 1
Qing Shao and Carol K. Hall

Probing How Defects in Self-assembled Monolayers Affect Peptide Adsorption with Molecular Simulation ................................................. 21
K.G. Sprenger, Yi He and Jim Pfaendtner

Development of a Coarse-Grained Water Forcefield via Multistate Iterative Boltzmann Inversion .............................................................. 37
Timothy C. Moore, Christopher R. Iacovella and Clare McCabe

Optimizing Molecular Models Through Force-Field Parameterization via the Efficient Combination of Modular Program Packages ........................................... 53
Marco Hülsmann, Karl N. Kirschner, Andreas Krämer, Doron D. Heinrich, Ottmar Krämer-Fuhrmann and Dirk Reith

A Hierarchical, Component Based Approach to Screening Properties of Soft Matter ................................................................. 79
Christoph Klein, János Sallai, Trevor J. Jones, Christopher R. Iacovella, Clare McCabe and Peter T. Cummings

Quantum Virial Coefficients via Path Integral Monte Carlo with Semi-classical Beads ................................................................. 93
Ramachandran Subramanian, Andrew J. Schultz and David A. Kofke

Homogeneous Nucleation of [dmin+]Cl– from its Supercooled Liquid Phase: A Molecular Simulation Study ............................................. 107
Xiaoxia He, Yan Shen, Francisco R. Hung and Erik E. Santiso
Influence of the Precursor Composition and Reaction Conditions
on Raney-Nickel Catalytic System ........................................ 125
Sabine Schweizer, Robin Chaudret, Theodora Spyriouni,
John Low and Lalitha Subramanian

Atomistic Modeling and Simulation for Solving Gas Extraction
Problems .................................................................................. 137
Genri E. Norman, Vasily V. Pisarev, Grigory S. Smirnov
and Vladimir V. Stegailov

Atomistic Simulations of CO2 During “Trapdoor” Adsorption
onto Na-Rho Zeolite ................................................................. 153
Nathan Bamberger and Daniela Kohen
Foundations of Molecular Modeling and Simulation
Select Papers from FOMMS 2015
Snurr, R.Q.; Adjiman, C.; Kofke, D.A. (Eds.)
2016, XIV, 168 p. 66 illus., 57 illus. in color., Hardcover
ISBN: 978-981-10-1126-9