

# Contents

<b>First-Principles-Based Multiscale, Multiparadigm Molecular Mechanics and Dynamics Methods for Describing Complex Chemical Processes .....</b>	<b>1</b>
Andres Jaramillo-Botero, Robert Nielsen, Ravi Abrol, Julius Su, Tod Pascal, Jonathan Mueller, and William A. Goddard III	
<b>Dynamic QM/MM: A Hybrid Approach to Simulating Gas-Liquid Interactions .....</b>	<b>43</b>
Scott Yockel and George C. Schatz	
<b>Multiscale Modelling in Computational Heterogeneous Catalysis .....</b>	<b>69</b>
F.J. Keil	
<b>Real-World Predictions from Ab Initio Molecular Dynamics Simulations .....</b>	<b>109</b>
Barbara Kirchner, Philipp J. di Dio, and Jürg Hutter	
<b>Nanoscale Wetting Under Electric Field from Molecular Simulations ..</b>	<b>155</b>
Christopher D. Daub, Dusan Bratko, and Alenka Luzar	
<b>Molecular Simulations of Retention in Chromatographic Systems: Use of Biased Monte Carlo Techniques to Access Multiple Time and Length Scales .....</b>	<b>181</b>
Jake L. Rafferty, J. Ilja Siepmann, and Mark R. Schure	
<b>Thermodynamic Properties for Applications in Chemical Industry via Classical Force Fields .....</b>	<b>201</b>
Gabriela Guevara-Carrion, Hans Hasse, and Jadran Vrabec	

<b>Multiscale Approaches and Perspectives to Modeling Aqueous Electrolytes and Polyelectrolytes</b> .....	251
Luigi Delle Site, Christian Holm, and Nico F.A. van der Vegt	
<b>Coarse-Grained Modeling for Macromolecular Chemistry</b> .....	295
Hossein Ali Karimi-Varzaneh and Florian Müller-Plathe	
<b>Index</b> .....	323

Multiscale Molecular Methods in Applied Chemistry

Kirchner, B.; Vrabec, J. (Eds.)

2012, XII, 328 p., Hardcover

ISBN: 978-3-642-24967-9