

Preface

Driven by advances in simulation methodology and computer hardware, an increasing spectrum of topics in applied chemistry is becoming accessible via the use of computational methods. In recent years, multiscale molecular simulations of complete and realistic processes have thereby emerged. This volume of *Topics in Current Chemistry* focuses on molecular methods for large and complex systems, such as technical chemical processes. It spans the spectrum from representative methodological approaches containing static quantum chemical calculations, ab initio molecular simulations, and traditional force field methods, to coarse-grained simulations from a multiscale perspective. Each field of theoretical chemistry is highly advanced, and although there is still room for further developments, these do not seem as tremendous as ten years ago if only one scale is considered. Current developments are often concerned with the refinement of old methods rather than with introducing new ones. Because the considered systems have become larger and more complex, the next step towards their accurate description lies in combining the advantages of more than one method, i.e. in multiscale approaches.

The multiscale aspect comes into play on different levels; one level is given by the well-known hybrid approach, i.e. combining existing methods in a concurrent calculation. Separate calculations applying different methods to the same system provide another approach. Coarser methods can be refined by more accurate methods and more accurate methods speeded up by making them more coarse. The investigated systems range from a single molecule to industrial processes. On the level of fluid properties, a scale-bridging ansatz considers molecular properties such as electronic energies, as well as thermodynamic quantities such as pressure. Thus, a connection between different levels is established. Furthermore, dynamic heterogeneity is accessible, and therefore a broader scale range in terms of dynamics can be covered. As microscopic movements on the femtosecond scale may substantially influence entire processes, the consequences for the macroscopic level are also taken into account.

The contributions to this volume cover applied topics such as hierarchically structured materials, molecular reaction dynamics, chemical catalysis, thermodynamics of aggregated phases, molecular self-assembly, chromatography, nanoscale

electrowetting, polyelectrolytes, charged colloids and macromolecules. Throughout, the authors have aimed at quantitative and qualitative predictions for complex systems in technical chemistry and thus in real-world applications. The nine chapters are structured in three groups: 1. *From first-principle calculations to complex systems via several routes* (Jaramillo-Botero et al., Yockel and Schatz, Keil, and Kirchner et al.), 2. *Making molecular dynamics simulations larger and accessing more complex situations* (Daub et al., Rafferty et al., and Guevara-Carrion et al.) and 3. *Coarse grained modelling reaching out afar* (Delle Site et al., and Karimi-Varzaneh and Müller-Plathe).

We would like to thank all the authors as well as all those who have facilitated this volume, and hope that readers will consider it as a helpful tool for obtaining an overview of the recent developments in the field of multiscale molecular methods in applied chemistry.

Leipzig and Paderborn

Barbara Kirchner
Jadran Vrabec

Multiscale Molecular Methods in Applied Chemistry

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

2012, XII, 328 p., Hardcover

ISBN: 978-3-642-24967-9