

Preface

This volume is based on my habilitation thesis (Habilitationsschrift) that was accepted from the Faculty of Mechanical Engineering of the Technische Universität Braunschweig for granting the *venia legendi* for the field of teaching “Molecular Thermodynamics”.

While my early research activities involved traditional experimental studies on thermophysical properties in the lab, I had the chance to perform first “computational experiments” during a research visit in the group of Richard Sadus. Since then I have focused my research on molecular simulations due to my fascination for its ability to allow for predictive studies and to gain insights into the systems on a molecular level that helps to interpret their properties. Shortly after I also started to teach a master course on molecular simulation. This course not only covers the fundamentals of molecular simulation, but also includes an introduction to the statistical mechanics that provide its theoretical framework, and details on force field models and their parametrization. This has motivated me to compose a comprehensive textbook that covers all these topics.

Molecular simulations have a wide range of application, but my research has always focused on studies on thermophysical properties. This is therefore also the scope of this volume, and it was important for me to devote a special chapter on the analysis of simulation outputs to derive different thermophysical properties. A main field of my research for the last years has been the molecular modeling and simulation for new HFO working fluids. These simulation studies are mainly described at the end of this textbook as illustrative example to demonstrate the ability of molecular simulations to provide predictions on the thermophysical properties of pure components and mixtures for which only limited experimental data are available.

Most of the simulation studies were performed at the Laboratory for Thermodynamics (IfT) of the Technische Universität Braunschweig, and I express my sincere gratitude to the head of the IfT, Jürgen Köhler, for enabling me to work in the fascinating research field of molecular simulation, and for his encouragement to accomplish this habilitation thesis (Habilitationsschrift). I’d also like to express my gratitude to Jadran Vrabec (ThEt, University Paderborn, Germany) and Hans

Hasse (LTD, TU Kaiserslautern, Germany) for agreeing to review this thesis, and I thank the members of the habilitation committee (Habilitationskommission) for their commitment.

I am grateful to all current and former colleagues, PhD students and graduate students from the IfT and TLK, who have somehow contributed to this thesis, for instance, by being involved in some molecular or system simulation studies, by reading versions of the text, by contributing figures for thermodynamics cycles etc.

As mentioned before, I had my first contact with molecular simulation during my stay at the Centre for Molecular Simulation of the Swinburne University in Hawthorn, Australia. I'm indebted to Richard Sadus and Billy Todd for introducing me to this research field, and for many fruitful discussions we have had since then. I especially want to thank Richard Sadus for his comments on this manuscript and for helpful suggestions.

The first stage of the force field for HFO/HCFO compounds, i.e. the model for fluorinated propenes, was developed during my stay in the group of Ed Maginn at the University of Notre Dame, USA. This stay was founded by a fellowship of the Deutsche Forschungsgemeinschaft (DFG). I appreciate this fellowship as it offered me the chance to spend some time in the group of Ed Maginn. I am grateful for his mentoring during my stay and since then. He influenced my work in various respects, and he deserves special thanks for many helpful and inspiring discussions, his support and encouragement. I'd also like to thank him for his valuable comments and helpful suggestions on several chapters of this manuscript. I am also indebted to Eric Lemmon, Arno Läsecke and Marcia Huber from the National Institute of Standard and Technology (NIST) in Boulder, USA, for providing the EOS and ECS models for the HFO and HCFO compounds that enabled the comparative REFPROP simulations, for helpful discussions and encouragement.

I'd also like to thank Ryo Akasaka (Kyushu Sangyo University, Fukuoka, Japan) and Katsuyuki Tanaka (Nihon University, Japan) for sharing their experimental data for the HFO and HCFO compounds with me, often prior to publication. Their data and EOS models allowed for a validation of the molecular model and the simulation results.

I reserve my deepest gratitude for my partner Jörg, for his support, encouragement and forbearance.

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