# Molecular Physical Chemistry for Engineers

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# Abbreviated Contents

# Contents

# Preface

This book is designed as a one-semester undergraduate course for engineers and materials scientists who need to understand physical chemistry. It responds to current trends in teaching this subject with a distinct emphasis on the behavior of matter from the molecular viewpoint. The book is focused on engineering students at the junior or senior level who have a background in beginning chemistry and physics and in beginning thermodynamics. A background in calculus and differential equations is assumed.

The products and processes that today's engineers and materials scientists create are increasingly based on concepts at the molecular level. This is true for "hard" materials such as semiconductors, alloys, ceramics, and polymer nanocomposites. It is also true for "soft" materials in areas of biocompatibility, biochemical engineering, and drug design. Traditional macroscopic thermodynamics and empirical equations of state often fail for nanoengineered materials and processes.

After a brief introductory review of basic thermodynamic functions, the book addresses only three core areas of physical chemistry: quantum chemistry, statistical mechanics, and kinetics. These areas form one core of modern physical chemistry and are closely linked with each other and with thermodynamics. A final chapter deals with case histories of the use of molecular modeling to solve engineering problems. The unification of the three core areas and their extension to some engineering applications may often be lost in physical chemistry courses aimed at students in the applied sciences, which are based on gigantic physical chemistry treatises.

We believe that the communication of concepts in physical science is often done best through the use of illustrations. Particularly in molecular-based sciences, the behavior of molecules can be illustrated in pictorial form with great effectiveness in teaching. Thus, this book is filled with drawings of molecular behavior, which illustrate the central concepts.

We wish to thank our wives, Kerin N. Yates and Linda Riding Johnson, for enduring the years associated with the writing of this book. Without their firm encouragement and sacrifice, the book would never have reached completion. JTY acknowledges with thanks the provision of a sabbatical leave from the University of Pittsburgh, which made the writing possible, and the full support of the project by Dean N. J. Cooper. JTY wishes to thank the Department of Chemistry at the University of Virginia for its grand hospitality in providing peace and quiet, as well as numerous important discussions about science and the book. In particular, Professor Ian Harrison has been a strong supporter of the writing efforts in many ways. The accurate and rapid secretarial work by Mrs. Margaret A. Augenstein, secretary to JTY, is recognized with thanks as a key resource for successfully producing this book. JKJ wishes to thank many colleagues at the University of Pittsburgh and the National Energy Technology Laboratory for helpful discussions and encouragement of this work. We gratefully acknowledge the help of Giovanni Garberoglio, who made many insightful and helpful suggestions, Oleg Byl for careful checking of the problems and help with the figures, Matthew LaBrosse and Prashant Kumar for carefully checking the manuscript, and Götz Veser for suggestions on Chapter 7. JKJ thanks Roger Cracknell (Shell), David Frurip (Dow Chemical), Joseph Golab (B.P. America), Michael Golombok (Shell), and Peter Gordon (ExxonMobil) for helpful discussions on Chapter 8. We thank Professor Robert Enick for early discussions about the need for this book. We are grateful to John Murdzek for his very skilled copyediting, and to Jennifer Uhlich and Christine Taylor for their talented production work. Finally, we thank Bruce Armbruster and Jane Ellis at University Science Books for their guidance and encouragement throughout the entire process.

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