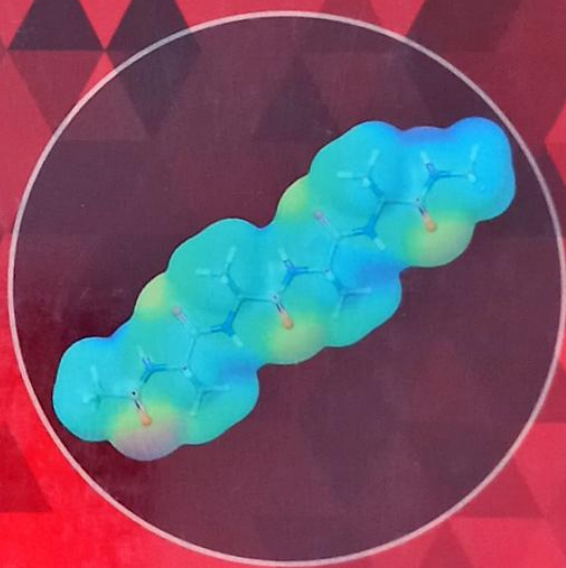# Introduction to
# **Computational**
# **Chemistry**



## Frank Jensen

# Introduction to Computational Chemistry

### Third Edition

*Frank Jensen*
*Department of Chemistry, Aarhus University, Denmark*

# WILEY

# Contents

## Third Edition

# Introduction to Computational Chemistry

**FRANK JENSEN** *Department of Chemistry, Aarhus University, Denmark*

Following on from the success of the second edition, *Introduction to Computational Chemistry, Third Edition*, provides an updated account of the fundamental principles underlying different methods, ranging from classical to sophisticated quantum models. Subjects covered include molecular structures and energetics, molecular properties, dynamic aspects, relative methods and qualitative models.

### New to this Edition

- Substantially revised throughout; methodologies and references in each chapter have been updated to reflect key developments since the second edition.
- New or expanded sections include force fields, density functional theory, excited states, time-dependent properties, accelerated dynamics, tensor decomposition and clustering methods.
- Includes more than 1000 references to reviews and original work.
- PowerPoint slides of all figures in the book are provided online.

An accessible introduction to the field, covering theory and practical aspects, this classic text is an invaluable guide for advanced undergraduates and graduate students entering the field of computational chemistry, as well as for professional researchers using computational methods as a tool for interpretations and designing new experiments and compounds.

**FRANK JENSEN** obtained his PhD from UCLA in 1987 with Professors C. S. Foote and K. N. Houk, and is currently an Associate Professor in the Department of Chemistry, Aarhus University, Denmark. He has published more than 150 papers and articles, and has made contributions to the widely used program package GAMESS.