Molecular Modeling of Geochemical Reactions. An Introduction

Description: Molecular processes in nature affect human health, the availability of resources and the Earth’s climate. Molecular modelling is a powerful and versatile toolbox that complements experimental data and provides insights where direct observation is not currently possible.

Molecular Modeling of Geochemical Reactions: An Introduction applies computational chemistry to geochemical problems. Chapters focus on geochemical applications in aqueous, petroleum, organic, environmental, bio- and isotope geochemistry, covering the fundamental theory, practical guidance on applying techniques, and extensive literature reviews in numerous geochemical sub-disciplines.

Topics covered include:
- Theory and Methods of Computational Chemistry
- Force Field Application and Development
- Computational Spectroscopy
- Thermodynamics
- Structure Determination
- Geochemical Kinetics

This book will be of interest to graduate students and researchers looking to understand geochemical processes on a molecular level. Novice practitioners of molecular modelling, experienced computational chemists, and experimentalists seeking to understand this field will all find information and knowledge of use in their research.

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