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.

Contents: List of Contributors xi

Preface xiii

1 Introduction to the Theory and Methods of Computational Chemistry 1
   David M. Sherman
   1.1 Introduction 1
   1.2 Essentials of Quantum Mechanics 2
     1.2.1 The Schrödinger Equation 4
     1.2.2 Fundamental Examples 4
   1.3 Multielectronic Atoms 7
     1.3.1 The Hartree and Hartree-Fock Approximations 7
     1.3.2 Density Functional Theory 13
   1.4 Bonding in Molecules and Solids 17
     1.4.1 The Born-Oppenheimer Approximation 17
     1.4.2 Basis Sets and the Linear Combination of Atomic Orbital Approximation 18
   1.5 From Quantum Chemistry to Thermodynamics 22
3 Quantum–Mechanical Modeling of Minerals 77
Alessandro Erba and Roberto Dovesi

3.1 Introduction 77
3.2 Theoretical Framework 79
3.2.1 Translation Invariance and Periodic Boundary Conditions 79
3.2.2 HF and KS Methods 80
3.2.3 Bloch Functions and Local BS 81
3.3 Structural Properties 82
3.3.1 P–V Relation Through Analytical Stress Tensor 83
3.3.2 P–V Relation Through Equation of State 85
3.4 Elastic Properties 86
3.4.1 Evaluation of the Elastic Tensor 86
3.4.2 Elastic Tensor–Related Properties 89
3.4.3 Directional Seismic Wave Velocities and Elastic Anisotropy 89
3.5 Vibrational and Thermodynamic Properties 91
3.5.1 Solid–State Thermodynamics 93
3.6 Modeling Solid Solutions 95
3.7 Future Challenges 98

References 99

4 First Principles Estimation of Geochemically Important Transition Metal Oxide Properties: Structure and Dynamics of the Bulk, Surface, and Mineral/Aqueous Fluid Interface 107
Ying Chen, Eric Bylaska, and John Weare

4.1 Introduction 107
4.2 Overview of the Theoretical Methods and Approximations Needed to Perform AIMD Calculations 109
4.3 Accuracy of Calculations for Observable Bulk Properties 113
4.3.1 Bulk Structural Properties 113
4.3.2 Bulk Electronic Structure Properties 118
4.4 Calculation of Surface Properties 123
4.4.1 Surface Structural Properties 123
4.4.2 Electronic Structure in the Surface Region 127
4.4.3 Water Adsorption on Surface 129
4.5 Simulations of the Mineral–Water Interface 130
4.5.1 CPMD Simulations of the Vibrational Structure of the Hematite (012) Water Interface 130
6.3 Applications 196

6.3.1 Modeling of Surface Complexes of Polar Phenoxyacetic Acid–Based Herbicides with Iron Oxyhydroxides and Clay Minerals 197

6.3.2 Modeling of Adsorption Processes of Polycyclic Aromatic Hydrocarbons on Iron Oxyhydroxides 217

6.3.3 Modeling of Interactions of Polar and Nonpolar Contaminants in Organic Geochemical Environment 220

6.4 Perspectives and Future Challenges 227

Glossary 229

References 231

7 Petroleum Geochemistry 245
Qisheng Ma and Yongchun Tang

7.1 Introduction: Petroleum Geochemistry and Basin Modeling 245

7.2 Technology Development of the Petroleum Geochemistry 246

7.2.1 Thermal Maturity and Vitrinite Reflectance 246

7.2.2 Rock-Eval Pyrolysis 247

7.2.3 Kerogen Pyrolysis and Gas Chromatography Analysis 248

7.2.4 Kinetic Modeling of Kerogen Pyrolysis 249

7.2.5 Natural Gases and C/H Isotopes 253

7.3 Computational Simulations in Petroleum Geochemistry 253

7.3.1 Ab Initio Calculations of the Unimolecular C–C Bond Rapture 253

7.3.2 Quantum Mechanical Calculations on Natural Gas 13C Isotopic Fractionation 256

7.3.3 Deuterium Isotope Fractionations of Natural Gas 258

7.3.4 Molecular Modeling of the 13C and D Doubly Substituted Methane Isotope 260

7.4 Summary 262

References 262

8 Mineral–Water Interaction 271
Marie-Pierre Gaigeot and Marialore Sulpizi

8.1 Introduction 271

8.2 Brief Review of AIMD Simulation Method 275

8.2.1 Ab Initio Molecular Dynamics and Density Functional Theory 275

8.3 Calculation of the Surface Acidity from Reversible Proton Insertion/Deletion 280

8.4 Theoretical Methodology for Vibrational Spectroscopy and Mode Assignments 282

8.5 Property Calculations from AIMD: Dipoles and Polarisabilities 284

8.6 Illustrations from Our Recent Works 286
8.6.1 Organisation of Water at Silica Water Interfaces: (0001) –Quartz Versus Amorphous Silica 286
8.6.2 Organisation of Water at Alumina Water Interface: (0001) –Alumina Versus (101) Boehmite 291
8.6.3 How Surface Acidities Dictate the Interfacial Water Structural Arrangement 293
8.6.4 Vibrational Spectroscopy at Oxide Liquid Water Interfaces 295
8.6.5 Clay Water Interface: Pyrophyllite and Calcium Silicate 299

8.7 Some Perspectives for Future Works 302

References 304

9 Biogeochemistry 311
Weilong Zhao, Zhijun Xu, and Nita Sahai

9.1 Introduction 311

9.1.1 Mineral Water Interactions 313
9.1.2 Mineral Organic Interactions 313

9.2 Challenges and Approaches to Computational Modeling of Biomineralization 314

9.2.1 Biominerals: Structure, Nucleation, and Growth 314
9.2.2 Conformational Sampling in Modeling Biomineralization 317
9.2.3 Force Field Benchmarking 324
9.2.4 Ab Initio MD and Hybrid QM/MM Approaches 325

9.3 Case Studies 326
9.3.1 Apatite 327
9.3.2 Calcite 331

9.4 Concluding Remarks and Future Perspectives 334

Acknowledgments 335

References 335

10 Vibrational Spectroscopy of Minerals Through Ab Initio Methods 341
Marco De La Pierre, Raffaella Demichelis, and Roberto Dovesi

10.1 Introduction 341

10.2 Theoretical Background and Methods 342

10.2.1 Calculation of Vibrational Frequencies 344
10.2.2 Splitting of the Longitudinal Optical (LO) and Transverse Optical (TO) Modes 346
10.2.3 Calculation of Infrared (IR) and Raman Peak Intensities and of the IR Dielectric Function 347
10.2.4 Estimation of the Anharmonic Constant for X H Stretching Modes 349
10.2.5 Accuracy of Basis Set and Hamiltonian 350
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