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Topics in Current Chemistry

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Aims and Scope

The series Topics in Current Chemistry presents critical reviews of the present and future trends in modern chemical research. The scope of coverage includes all areas of chemical science including the interfaces with related disciplines such as biology, medicine and materials science.

The goal of each thematic volume is to give the non-specialist reader, whether at the university or in industry, a comprehensive overview of an area where new insights are emerging that are of interest to larger scientific audience.

Thus each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole. The most significant developments of the last 5 to 10 years should be presented. A description of the laboratory procedures involved is often useful to the reader. The coverage should not be exhaustive in data, but should rather be conceptual, concentrating on the methodological thinking that will allow the non-specialist reader to understand the information presented.

Discussion of possible future research directions in the area is welcome.

Review articles for the individual volumes are invited by the volume editors.

Readership: research chemists at universities or in industry, graduate students.

Şule Atahan-Evrenk • Alán Aspuru-Guzik
Editors

Prediction and Calculation of Crystal Structures

Methods and Applications

With contributions by

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Preface

The prediction of crystal structure for a chemical compound is still a challenge. It requires advanced algorithms for exhaustive searches of the possible packing forms and highly accurate computational methodologies to rank the possible crystal structures. This book presents some of the important developments in crystal structure prediction in recent years. The chapters do not cover every area but rather present a wide range of methodologies with applications in organic, inorganic, and hybrid compounds.

The blind tests organized by the Cambridge Crystallographic Data Center (CCDC) showed a notable improvement for the crystal structure prediction of organic compounds over recent years. The first two chapters of this book present two of the methodologies contributed to the success in recent blind tests. The chapter "Dispersion Corrected Hartree–Fock and Density Functional Theory for Organic Crystal Structure Prediction" by Brandenburg and Grimme is dedicated to recent advances in the dispersion-corrected Hartree–Fock and density functional theory. Another important area showing remarkable progress is the efficient treatment of the internal flexibility of molecules with many rotatable bonds. The chapter "General Computational Algorithms for Ab Initio Crystal Structure Prediction for Organic Molecules" by Pantelides et al. summarizes some of the algorithms that have contributed to this success. In addition, the chapter "Accurate and Robust Molecular Crystal Predictions Using Fragment-Based Electronic Structure Methods" by Beran et al. illustrates how fragment-based electronic structure methods can provide accurate prediction of the lattice energy differences of polymorphs of organic compounds.

One research area that would benefit tremendously from the crystal structure prediction of organic compounds is the design of organic semiconductors. In the chapter "Prediction and Theoretical Characterization of Organic Semiconductor Crystals for Field-Effect Transistor Applications" by Şule Atahan-Evrenk and Alán Aspuru-Guzik, discuss some aspects of theoretical characterization and prediction of crystal structures of p-type organic semiconductors for organic transistor applications. The chapter also provides information about the structure–property relationships in organic semiconductors.

In organic systems, thanks to the internal constraints of molecular structures, random sampling methods can be used successfully. In inorganic crystals, however, there are no constraints other than the chemical compositions. Therefore, the challenge in the crystal structure prediction of inorganic compounds is the search problem, and the methodologies that span the search space effectively are crucial. The chapters by Hautier, by Revard et al., and by Zhu et al. are dedicated to cover recent advances towards achieving inorganic crystal prediction. The chapter "Data Mining Approaches to High-Throughput Crystal Structure and Compound Prediction" by Hautier discusses data mining approaches and the chapters by Revard et al. and by Zhu et al. cover evolutionary algorithms for compound prediction. In particular, the chapter "Structure and Stability Prediction of Compounds with Evolutionary Algorithms" by Revard et al. presents different methodologies adapted for the evolutionary algorithms approaches and the chapter "Crystal Structure Prediction and Its Application in Earth and Materials Sciences" by Zhua et al. focuses on the state of the art of the USPEX methodology.

The prediction of hybrid materials such as metal-organic frameworks posits a specific set of challenges for structure prediction. The chapter "Large-Scale Generation and Screening of Hypothetical Metal-Organic Frameworks for Applications in Gas Storage and Separation" by Wilmer and Snurr discusses the large-scale generation and screening of metal-organic frameworks. With possible applications in storage, catalysis, pharmaceuticals, and electrochemistry, these methodologies show great potential for development of hybrid systems.

We believe crystal structure prediction will be one of the most important tools in solid-state chemistry in the near future. Applications ranging from pharmaceuticals to energy technologies would benefit tremendously from computational prediction of the solid forms of materials. We believe this book provides up-to-date, concise, and accessible coverage of the subject for a wide audience in academia and industry and we hope that it will be useful for chemists and materials scientists who want to learn more about the state-of-the-art in crystal structure prediction methods and applications.

We would like to thank Springer editors Birke Dalia and Elizabeth Hawkins for inviting us to edit this volume and all the authors for their contributions. Lastly, we would like to thank all the members of the Aspuru-Guzik Group for their support and camaraderie.

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