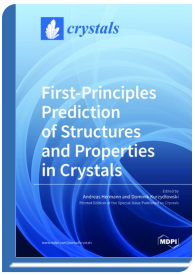
crystals

IMPACT FACTOR 2.7

CITESCORE 3.6

Special Issue Reprint

First-Principles Prediction of Structures and Properties in Crystals



www.mdpi.com/books/reprint/1746

Edited by
Andreas Hermann
Dominik Kurzydlowski

ISBN 978-3-03921-670-3 (Softback)
ISBN 978-3-03921-671-0 (PDF)

The term “first-principles calculations” is a synonym for the numerical determination of the electronic structure of atoms, molecules, clusters, or materials from ‘first principles’, i.e., without any approximations to the underlying quantum-mechanical equations.

Although numerous approximate approaches have been developed for small molecular systems since the late 1920s, it was not until the advent of the density functional theory (DFT) in the 1960s that accurate “first-principles” calculations could be conducted for crystalline materials. The rapid development of this method over the past two decades allowed it to evolve from an explanatory to a truly predictive tool.

Yet, challenges remain: complex chemical compositions, variable external conditions (such as pressure), defects, or properties that rely on collective excitations—all represent computational and/or methodological bottlenecks. This Special Issue comprises a collection of papers that use DFT to tackle some of these challenges and thus highlight what can (and cannot yet) be achieved using first-principles calculations of crystals.

MDPI

Order Your Print Copy
You can order print copies at
www.mdpi.com/books/reprint/1746

MDPI Books

Publishing Open Access Books & Series

MDPI Books offers quality open access book publishing to promote the exchange of ideas and knowledge in a globalized world. MDPI Books encompasses all the benefits of open access – high availability and visibility, as well as wide and rapid dissemination. With MDPI Books, you can complement the digital version of your work with a high quality printed counterpart.

Open Access

Your scholarly work is accessible worldwide without any restrictions. All authors retain the copyright for their work distributed under the terms of the Creative Commons Attribution License.

Author Focus

Authors and editors profit from MDPI's over two decades of experience in open access publishing, our customized personal support throughout the entire publication process, and competitive processing charges as well as unique contributor discounts on book purchases.

High Quality & Rapid Publication

MDPI ensures a thorough review for all published items and provides a fast publication procedure. State-of-the-art research and time-sensitive topics are released with a minimum amount of delay.

High Visibility

Due to our global network and well-known channel partners, we ensure maximum visibility and broad dissemination. Title information of books is sent to international indexing databases and archives, such as the Directory of Open Access Books (DOAB), and the Verzeichnis Lieferbarer Bücher (VLB).

Print on Demand and Multiple Formats

MDPI Books are available for purchase and to read online at any time. Our print-on-demand service offers a sustainable, cost-effective and fast way to publish MDPI Books printed versions.

MDPI AG
St. Alban-Anlage 66
4052 Basel
Switzerland
Tel: +41 61 683 77 34
www.mdpi.com/books
books@mdpi.com