Structure and Bonding 147

Electron Density and Chemical Bonding II

Theoretical Charge Density Studies

Bearbeitet von
Dietmar Stalke

1. Auflage 2012. Buch. xiv, 290 S. Hardcover
ISBN 978 3 642 30807 9
Format (B x L): 15,5 x 23,5 cm
Gewicht: 619 g

Weitere Fachgebiete > Chemie, Biowissenschaften, Agrarwissenschaften > Chemie Allgemein

schnell und portofrei erhältlich bei

beck-shop.de
DIE FACHBUCHHANDLUNG

Die Online-Fachbuchhandlung beck-shop.de ist spezialisiert auf Fachbücher, insbesondere Recht, Steuern und Wirtschaft. Im Sortiment finden Sie alle Medien (Bücher, Zeitschriften, CDs, eBooks, etc.) aller Verlage. Ergänzt wird das Programm durch Services wie Neuerscheinungsdienst oder Zusammenstellungen von Büchern zu Sonderpreisen. Der Shop führt mehr als 8 Millionen Produkte.

Preface

The electron density distribution is the ultimate observable for determining and interpreting the properties of matter. Analysing the electron density and assigning its features to properties will inevitably provide routes to rationally modifying the desired properties of matter in a predictable manner. Fortunately, the electron density may be analysed in two different and independent ways: firstly from quantum theory which leads to the molecular wave functions and secondly from the diffraction experiment. Therefore, ambiguities possibly introduced from model bias may be minimized by reference to both sets of data. Results obtained from X-ray diffraction which are subject to experimental errors may be validated by those obtained from theoretical methods. Conversely, new theoretical approaches inherently limited by computer power and memory size can be bench-marked using data from diffraction experiments.

The collection of review articles published in Volumes 146 and 147 of the Structure and Bonding Series provides a state-of-the-art overview of the experimental and theoretical determination of charge densities written by leaders in the field. We hope that their insights will motivate more scientists to take advantage of the approach.

Göttingen
April 2012

Dietmar Stalke

Springer

http://www.springer.com/978-3-642-30807-9

Electron Density and Chemical Bonding II
Theoretical Charge Density Studies
(Ed.)D. Stalke
2012, XIII, 289 p. 63 illus., 54 in color., Hardcover
ISBN: 978-3-642-30807-9