

Carlo Gatti • Piero Macchi
Editors

Modern Charge-Density Analysis

 Springer

Contents

1	A Guided Tour Through Modern Charge Density Analysis	1
	Carlo Gatti and Piero Macchi	
2	Electron Densities and Related Properties from the <i>ab-initio</i> Simulation of Crystalline Solids	79
	Cesare Pisani, Roberto Dovesi, Alessandro Erba, and Paolo Giannozzi	
3	Modeling and Analysing Thermal Motion in Experimental Charge Density Studies	133
	Anders Ø. Madsen	
4	Spin and the Complementary Worlds of Electron Position and Momentum Densities	165
	Jonathan A. Duffy and Malcom J. Cooper	
5	Past, Present and Future of Charge Density and Density Matrix Refinements	181
	Jean-Michel Gillet and Tibor Koritsanszky	
6	Using Wavefunctions to Get More Information Out of Diffraction Experiments	213
	Dylan Jayatilaka	
7	Local Models for Joint Position and Momentum Density Studies	259
	Jean-Michel Gillet	
8	Magnetization Densities in Material Science	277
	Béatrice Gillon and Pierre Becker	
9	Beyond Standard Charge Density Topological Analyses	303
	Angel Martín Pendás, Miroslav Kohout, Miguel Alvarez Blanco, and Evelio Francisco	

10	On the Interplay Between Real and Reciprocal Space Properties	359
	Wolfgang Scherer, Georg Eickerling, Christoph Hauf, Manuel Presnitz, Ernst-Wilhelm Scheidt, Volker Eyert, and Rainer Pöttgen	
11	Intermolecular Interaction Energies from Experimental Charge Density Studies	387
	Paulina M. Dominiak, Enrique Espinosa, and János G. Ángyán	
12	Chemical Information from Charge Density Studies	435
	Ulrike Flierler, Dietmar Stalke, and Louis J. Farrugia	
13	Charge Density in Materials and Energy Science	469
	Jacob Overgaard, Yuri Grin, Masaki Takata, and Bo B. Iversen	
14	A Generic Force Field Based on Quantum Chemical Topology	505
	Paul L.A. Popelier	
15	Frontier Applications of Experimental Charge Density and Electrostatics to Bio-macromolecules	527
	Christian Jelsch, Sławomir Domagała, Benoît Guillot, Dorothee Liebschner, Bertrand Fournier, Virginie Pichon-Pesme, and Claude Lecomte	
16	Charge Densities and Crystal Engineering	553
	Mark A. Spackman	
17	Electron Density Topology of Crystalline Solids at High Pressure	573
	John S. Tse and Elena V. Boldyreva	
18	Bonding Changes Along Solid-Solid Phase Transitions Using the Electron Localization Function Approach	625
	Julia Contreras-García, Miriam Marqués, Bernard Silvi, and José M. Recio	
19	Multi-temperature Electron Density Studies	659
	Riccardo Destro, Leonardo Lo Presti, Raffaella Soave, and Andrés E. Goeta	
20	Transient Charge Density Maps from Femtosecond X-Ray Diffraction	697
	Thomas Elsaesser and Michael Woerner	
21	Charge Density and Chemical Reactions: A Unified View from Conceptual DFT	715
	Paul A. Johnson, Libero J. Bartolotti, Paul W. Ayers, Tim Fievez, and Paul Geerlings	
	Index	765