

# Contents

## Preface — V

## Part I: The importance of chemical bonding concepts

Simon Grabowsky

- 1      **Introduction to complementary bonding analysis — 3**

Dietmar Stalke

- 2      **Chemical concepts of bonding and current research problems, or: Why should we bother to engage in chemical bonding analysis? — 9**

## Part II: Bonding descriptors from quantum chemistry

Ángel Martín Pendás and Carlo Gatti

- 3      **Quantum theory of atoms in molecules and the AIMAll software — 43**

Miroslav Kohout

- 4      **Electron localizability indicator and bonding analysis with DGrid — 75**

Jean Christophe Tremblay

- 5      **Is there a unique way of localizing molecular orbitals, and why not — 113**

Eric D. Glendening, Clark R. Landis, and Frank Weinhold

- 6      **Natural bond orbital theory: Discovering chemistry with NBO7 — 129**

Avital Shurki, Benoît Braïda, and Wei Wu

- 7      **Valence bond theory with XMVB — 157**

Trevor A. Hamlin, Pascal Vermeeren, Célia Fonseca Guerra, and F. Matthias Bickelhaupt

- 8      **Energy decomposition analysis in the context of quantitative molecular orbital theory — 199**

## Part III: Bonding descriptors from quantum crystallography

Piero Macchi

- 9      **Introduction to quantum crystallography — 215**

Benoît Guillot, Christian Jelsch, and Piero Macchi	Contents
<b>10 Multipole modeling with MoPro and XD — 235</b>	Part I: The importance of chemical periodicity
Alessandro Genoni and Dylan Jayatilaka	Periodicities
<b>11 X-ray constrained wavefunction analysis with Tonto — 269</b>	Periodicities
Dana Nachtigallová and Pavel Hobza	Periodicities
<b>12 Introduction to noncovalent interactions — 309</b>	Noncovalent interactions
Mark A. Spackman, Peter R. Spackman, and Sajesh P. Thomas	Noncovalent interactions
<b>13 Beyond Hirshfeld surface analysis: Interaction energies, energy frameworks and lattice energies with <i>CrystalExplorer</i> — 329</b>	Noncovalent interactions
Rubén Laplaza, Francesca Peccati, David Arias-Olivares, and Julia Contreras-García	Part II: Bonding descriptions from quantum chemistry
<b>14 Visualizing non-covalent interactions with NCIPILOT — 353</b>	Visualizations
<b>Appendix — 379</b>	Appendix
<b>Index — 383</b>	Index