## Contents

### Part I Condensed Matter Theory

1. **Can the $d$-Orbital Splitting Unveil the Local Structure of Cu$^{2+}$ Ions? Study on the $K_2ZnF_4$·Cu$^{2+}$ Archetype**
   - Fernando Rodríguez
   - Page 3

2. **Introducing the Inner Structure of the Magnetic Atom in the Interaction Between a Transition Metal Atom Impurity and a Metal Surface**
   - Fernando Flores and E.C. Goldberg
   - Page 17

3. **Structural Effects on Electronic Properties of Selected Materials**
   - G.G.N. Angilella
   - Page 31

4. **Anomalous Magnetism and Superconductivity in Lanthanide Metals at Extreme Pressure**
   - James S. Schilling
   - Page 47

5. **Phonon Fingerprints on Low and High-Energy Spectrum of Cuprate Superconductors**
   - R. Citro
   - Page 57

6. **Electrides and Their High-Pressure Chemistry**
   - Xiao Dong and Artem R. Oganov
   - Page 69

   - C.C. Matthai and N.H. March
   - Page 85

8. **Equations of State for Solids Under Strong Compression with Fingerprints for Electronic Anomalies**
   - Wilfried B. Holzapfel
   - Page 91
9 Band Gaps and Effective Oscillator Models for Solid Hydrogen and H₂O Ice at High Pressure .................................. 107
Wai-Leung Yim, Hongliang Shi, Yunfeng Liang,
Russell J. Hemley and John S. Tse

10 Nonequilibrium Steady States and Electron Transport
in Molecular Systems .................................................. 127
I. Deretzis, S.F. Lombardo, G.G.N. Angilella, R. Pucci
and A. La Magna

11 Peierls and Spin-Density Instability: From Polyacetylene
to Graphene .......................................................... 151
M. Baldo

12 Generalized Dicke Model of Graphene Cavity QED ............ 167
F.M.D. Pellegrino

13 A Comparison Between Quantum Transport and Band
Structure Unfolding in Defected Graphene Nanoribbons .......... 185
I. Deretzis and A. La Magna

14 Defect-Induced Magnetism in Graphene: An Ab Initio Study..... 195
A. Pidatella and R. Mazzarello

15 Electron Correlations in Molecular Chains ......................... 215
L.S. Brizhik

16 Hydrogen-Bonded Systems Under Intense Electric Fields .......... 233
G. Cassone, F. Saija, A.M. Saitta and P.V. Giaquinta

17 Miniature Spherical Sapphire Anvil Cell for Small
Angle Neutron Scattering ............................................. 247
X. Wang, N.A. Parzyk, D.M. Paul, C.D. Dewhurst,
G. Giriat and K.V. Kamenev

18 Are Light Alkali Metals Still Metals Under High Pressure? .... 257
F. Siringo, R. Pucci and G.G.N. Angilella

Part II Molecular Chemistry

19 Negative Condensed-to-Atom Fukui Functions: A Signature
of Oxidation-Induced Reduction of Functional Groups ............ 269
E. Echegaray, A. Toro-Labbe, K. Dikmenli, F. Heidar-Zadeh,
N. Rabi, S. Rabi, P.W. Ayers, C. Cardenas,
Robert G. Parr and J.S.M. Anderson

20 Simple Approaches to Calculate Correlation Energy
in Polyatomic Molecular Systems ..................................... 279
A. Grassi, G.M. Lombardo and G. Forte
R. Pucci

22 Electron Density, Kohn–Sham Frontier Orbitals, and Fukui Functions ........................................... 303
Weitao Yang, Robert G. Parr and R. Pucci

Part III Theoretical Physics

23 From Condensed Matter to QCD: A Journey Through Gauge Theories on Board of a Variational Tool ............... 309
Fabio Siringo

Part IV Philosophy and History of Science

24 The Languages of Science, Religion, and Theology ............ 331
G. Ruggieri

25 Symmetries and Physics ........................................ 345
R. Pucci

26 Science and Religion: A Difficult Relationship ................. 359
R. Pucci and G.G.N. Angilella

27 The Bold and the Humble: Physics and Epistemology .......... 369
R. Pucci and G.G.N. Angilella

28 Ettore Majorana’s Early Scientific Production ................. 373
R. Pucci and G.G.N. Angilella

29 Einstein and His Struggle for Peace .......................... 391
R. Pucci and G.G.N. Angilella

Author Index .................................................. 397

Subject Index .................................................. 399
Correlations in Condensed Matter under Extreme Conditions
A tribute to Renato Pucci on the occasion of his 70th birthday
Angilella, G.G.N.; La Magna, A. (Eds.)
2017, XVI, 401 p. 126 illus., Hardcover
ISBN: 978-3-319-53663-7