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Descrizione fisica	1 online resource (248 pages)
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Nota di contenuto	Frontmatter -- Preface -- Contents -- List of Contributing authors -- 1. Optical properties of monolayer BeC under an external electric field: A DFT approach / Chowdhury, Suman / Jana, Debnarayan -- 2. Theoretical investigation of the derivatives of favipiravir (T-705) as potential drugs for Ebola virus / Rhyman, Lydia / Tursun, Mahir / Abdallah, Hassan H. / Choong, Yee Siew / Parlak, Cemal / Kharkar, Prashant / Ramasami, Ponnadurai -- 3. Potential thermally activated delayed fluorescence properties of a series of 2,3-dicyanopyrazine based compounds / Gümü, Ayegül / Gümü, Selçuk -- 4. -Al2O3: Ce3+Cu2+ as a phosphor material; DFT+U and experimental approach -- 5. A DFT perspective analysis of optical properties of defected germanene mono-layer / Dhar, Namrata / Jana, Debnarayan -- 6. DFT studies on storage and adsorption capacities of gases on MOFs / Gulati, Archa / Kakkar, Rita -- 7. Metastability of the boron-vacancy complex in silicon: Insights from hybrid functional calculations / Ouma, Cecil N.M. / Meyer, Walter E. -- 8. Molecular structure and vibrational spectra of 2-(4-bromophenyl)-3-(4-hydroxyphenyl) 1,3-thiazolidin-4-one and its selenium analogue: Insights using HF and DFT methods / Kavitha, Helen P. / Rhyman, Lydia / Ramasami, Ponnadurai -- 9. Complexes between core-modified porphyrins ZnP(X)4 (X = P and S) and small semiconductor nanoparticle Zn6S6: are they possible? / Kuznetsov, Aleksey E. -- 10. DFT computations on vibrational spectra:

	Scaling procedures to improve the wavenumbers / Palafox, M. Alcolea -- 11. Substituent effects on linear and nonlinear optical properties of fluorescent (E)-2-(4-halophenyl)-7- arlstyrylimidazo[1,2-A] pyridine: spectroscopic and computational methods / Jadhav, Siddheshwar D. / Ramasami, Ponnadurai / Sekar, Nagaiyan -- Index
Sommario/riassunto	DFT methods are widely used in a broad range of disciplines to investigate many body systems. This book provides an overview on contemporary applications of the Density Functional Theory in various fields as computational chemistry, physics or engineering.