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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. -Al ₂ O ₃ : Ce ³⁺ +Cu ²⁺ 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 Zn ₆ S ₆ : are they possible? / Kuznetsov, Aleksey E. -- 10. DFT computations on vibrational spectra:

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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.
