

1. Record Nr.	UNINA9910467474003321
Titolo	Density functional theory : advances in applications // edited by Ponnadurai Ramasami
Pubbl/distr/stampa	Berlin ; ; Boston, Massachusetts : , : De Gruyter, , [2019] ©2019
ISBN	3-11-056695-8 3-11-056819-5
Descrizione fisica	1 online resource (248 pages)
Disciplina	523.112
Soggetti	Density wave theory Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
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:
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
