

1. Record Nr.	UNINA9910537030503321
Titolo	Computational sciences / / edited by Ponnadurai Ramasami
Pubbl/distr/stampa	Berlin, [Germany] ; ; Boston, [Massachusetts] : , : De Gruyter, , 2017 ©2017
ISBN	3-11-046548-5 3-11-046721-6
Descrizione fisica	1 online resource (236 pages) : illustrations
Disciplina	620.0028/5
Soggetti	Engineering - Data processing Research - Data processing Computer science Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	Frontmatter -- Preface of the Book of Proceedings of the Virtual Conference on Computational Science (VCCS-2016) -- Contents -- List of contributing authors -- 1. Addressing the challenges of standalone multi-core simulations in molecular dynamics / Ocaya, R.O. / Terblans, J.J. -- 2. Optical and magnetic properties of free-standing silicene, germanene and T-graphene system / Chowdhury, Suman / Bandyopadhyay, Arka / Dhar, Namrata / Jana, Debnarayan -- 3. Theoretical study of the electronic states of newly detected dications. Case of MgS ₂ ⁺ AND SiN ₂ ⁺ / Khairat, Toufik / Salah, Mohammed / Marakchi, Khadija / Komiha, Najia -- 4. Analytical Solution of Pantograph Equation with Incommensurate Delay / Patade, Jayvant / Bhalekar, Sachin -- 5. Computational chemistry applied to vibrational spectroscopy: A tool for characterization of nucleic acid bases and some of their 5-substituted derivatives / Palafox, M. Alcolea -- 6. Mechanism of nucleophilic substitution reactions of 4-(4'-nitro) phenylnitrobenzofurazan ether with aniline in acetonitrile / Gbayo, K. / Isanbor, C. / Lobb, K. / Oloba-Whenu, O. -- 7. Computational methods in preformulation study for pharmaceutical solid dosage forms of

therapeutic proteins / Majee, Sutapa Biswas / Biswas, Gopa Roy -- 8. Computational Investigation of Cationic, Anionic and Neutral Ag₂AuN (N = 1-7) Nanoalloy Clusters / Ranjan, Prabhat / Chakraborty, Tanmoy / Kumar, Ajay -- 9. Evacuation simulation using Hybrid Space Discretisation and Application to Large Underground Rail Tunnel Station / Chooramun, N / Lawrence, P. J. / Galea, E. R. -- 10. DFT study of anthocyanidin and anthocyanin pigments for Dye-Sensitized Solar Cells: Electron injecting from the excited states and adsorption onto TiO₂ (anatase) surface / Marcano, Emildo -- 11. Elemental Two-Dimensional Materials Beyond Graphene / Schwingenschlögl, Udo / Zhu, Jiajie / Morishita, Tetsuya / Spencer, Michelle J.S. / Padova, Paola De / Generosi, Amanda / Paci, Barbara / Ottaviani, Carlo / Quaresima, Claudio / Olivieri, Bruno / Salomon, Eric / Angot, Thierry / Lay, Guy Le / Zandvliet, Harold J.W. / Voon, L. C. Lew Yan -- Index

Sommario/riassunto

Eleven carefully selected, peer-reviewed contributions from the Virtual Conference on Computational Science (VCCS-2016) are featured in this edited book of proceedings. VCCS-2016, an annual meeting, was held online from 1st to 31st August 2016. The theme of the conference was "Computational Thinking for the Advancement of Society" and it matched the paradigm shift in the way we think. VCCS-2016 was attended by 100 participants from 20 countries. The chapters reflect a wide range of fundamental and applied research applying computational methods.
