Programme of VCCC-2014

1-31 August 2014

Date August 2014	Corresponding Author/s	Title
1	M. Zeema and P. Ramasami	International Year of Crystallography (IYCr2014)
Keynote E-Presentations		
2	J. Barroso-Flores	Reluctance towards Aromatization of Vinamidine Analogues into Substituted Pyridines. A Theoretical Evaluation of the Reaction Mechanisms that Never were
3	M. F. Bickelhaupt	Supramolecular Quantum Chemistry - From DNA Base Pairs *via* Nanoswitches to Remote Communication
4	M. Coote	Manipulating Stability and Orbital Configuration of Free Radicals with pH
5	R. Kakkar	Assessment of Molecular Binding of Hoechst 33258 Analogues into DNA using Docking and MM/GBSA Approach
6	A. Klamt	COSMO Polarization Charge Densities as Good Descriptors for the Quantification of Hydrogen Bond Enthalpy and Free Energy in Solution
7	P. Politzer and J. S. Murray	σ-Hole Interactions: A Physical Interpretation
8	N. Sekar	Red Emitting Coumarins: Insights of Photophysical Properties with DFT Calculations
Invited E-Presentations		
9	S. Abdalla	Theoretical Study of Substituted Pyrrolidines and Phospholanes in Gas Phase and Aqueous Phases
10	H. H. Abdallah	Theoretical Study on the Mechanism of 1,3-Dipolar Cycloaddition Reactions between α,β-Unsaturated Selenoaldehyde with Nitrone and Nitrile Oxide
11	K. Arora	3D-QSAR Studies for some Pyrazolones against a Pathogen
12	**Schrödinger Day**	
13	P. Kharkar	In Search of Novel Anti-Inflammatory Agents: Computational Repositioning of Approved Drugs
14	H. Bhakhoa	The Journey to Cyclen Complexes of Alkali Metal Azides

15	**Break**	
16	T. Chakraborty	A Theoretical Analysis of Bi-Metallic $(Cu\text{-}Ag)_{n = 1\text{-}7}$ Nano Alloy Clusters Invoking DFT Based Descriptors
17	C. S. Chidan Kumar	Molecular Structure, FT-IR, Raman, XRD and Quantum Chemical Studies of 2-Acetyl-5-chlorothiophene
18	S. Dhail	QSAR Study of Derivatives for Antimicrobial Evaluation of Novel Benzimidazole Type of Fluconazole Analogues Invoking Quantum Mechanical Based Descriptor
19	W. F. Gtari and B. Tangour	A Theoretical Study of the Dihydrogen Molecule Confined inside Carbon Nanotubes
20	T. Chakraborty	A Comparative Study of Different DFT Based Methodologies of Bi-Metallic $Ag\text{-}Au_{n\ (n=1\text{-}7)}$ Nano Alloy Clusters
21	R. Kakkar	Adsorption of Sarin on MgO Nanotubes: Roles of Doped and Defect Sites
22	D. Kumar Rawat	Structural Insight into Impact of Polymorphism on Vacuum Morphologies and Solubility Prediction of Felodipine Form IV
23	A. Kuznetsov	Metalloporphyrins with all the Pyrrole Nitrogens Replaced with Phosphorus Atoms, $MP(P)_4$ (M = Sc, Ti, Fe, Ni, Cu, Zn)
24	J. Z. A. Laloo	Theoretical Study of S_N2 Reactions
25	E. Marcano	Static (Hyper)Polarizability and Reorganization Energy of 4,5-Dicyanoimidazole
26	F. D. P. Morisso	Application of *Ab initio* Calculations on the Study of the Tanning Process
27	G. Roos	The Motor behind the Thiol/Disulfide Redox Potential is the Release of Conformational Strain
28	M. K. Singh	DFT Augmented Exploration of Rearrangement of Imidazole *N*-Oxide to Imidazole-2-ones in Aqueous Media
29	M. Szelag	Comparative Screening and Validation of a Novel Tool to Identify STAT-Specific Inhibitors
30	B. Tangour	Nanotubes: A Confinement Space to Store and to Activate Molecules
31	**Cultural Day/Follow Up**	