Poster Session I
Tuesday 27th July ; 17:30-20:00

Assigned topic	Subm. ID	Abstract title	Presenter
1. Conceptual DFT	51	Characterization of correlation-bound anions of perfluorinated molecules	TITECA, Charlotte
	59	Exploring The Reactivity Through a Conceptual and Constrained DFT Approach	PILMÉ, Julien
	93	Analysis of nearly planar defects using the Thomas–Fermi–von Weizsäcker model	KUMAR, Dharamveer
	95	Should electronic delocalization be associated with aromaticity?	SORIANO-AGUEDA, Luis
	143	Evaluation of non-covalent interactions with double-hybrid functional	MASSAFRA, Davide
2. DFT and condensed phases	24	Inducing out-of-plane magnetocrystalline anisotropy in 2D CuCrP2S6 by doping.	YADAV, Anita
	33	Strengthening Ni-based superalloys by γ-γ' partitioning regulation of Ta-W/Mo	ZHAO, Wenyue
	45	2D MA2Z4 vdW heterostructure for high-performing solar cell from DFT calculation	LIRA, Renan
	55	Exploring lubricant chemistry: From molecular dynamics to linear-scaling DFT	SARPA, Davide
	73	Synergistic Insights into the Tungsten-Tantalum-Vacancy System: A DFT-CE Study	PANDEY, Dhanshree
	76	Study of orientational relaxation of glass forming liquids	BISWAS, Biswarup
	80	Modelling the Lithium Anode-Electrolyte Interface under Potentiostatic control	AYERS, Brad
	83	DFT search for point defects in semiconductors for quantum devices	ABRIKOSOV, Igor
	85	Ab initio study of cyanide photo-dissociation/-association in a single crystal	MALEC, Leszek
	91	Role of N Diffusion Kinetics in Creating an Atomically Graded Ti/TiN interface	CHINNA VARALAKSHMI, Jalligampala
	105	Computational predictions of Pt(II)-based crystal structures and their emissions	NIEDZIELSKI, Grzegorz
	138	When the room is the elephant: chemical environment in DFT calculations	TURELLI, Michele
3. DFT and reactivity	13	Two best-of-both-worlds approaches to dissociative chemisorption on metals	KROES, Geert-Jan
	23	DFT study on the mechanism of site-selective acetate assisted C-H activation	APALOO-MESSAN, Edmond
	42	Exploring Resveratrol Photochemistry and Photodynamic Therapy Potential	YOSHINAGA, Mariana
	46	DFT study of conformers of Haloacetic Acid using Energy Decomposition Analysis	SEO, Wonil
	54	DFT Investigation of Stability of F2XNY (X = P, As, and Sb; Y = S, Se, and Te)	KIM, Joonghan
	70	Unraveling The Degradation Mechanism of Gentisic Acid Catalyzed by GDO Enzyme	NATH, Rounak
	94	A Combination of DFT and Spectroscopy to Solve Photocatalytic Mechanisms	NICOLAS, Emmanuel
	98	A theoretical study on the reaction of ethynyl radical with cyclopentadiene	CHANG, Agnes
	108	DFT for Organic Chemistry: Tackling the Challenges of Small and Large Molecules	MARYASIN, Boris
	156	Enlightening the reaction mechanism of furimazine oxidation in DMSO	BONARDI, Alessandro
4. Methodological Developments in DFT	16	Unveiling Thermoelectric Potential: Silver Chalcopyrites and DDH Approach	RANI, Dimple
	17	Non-empirical local range separation: Accurate excitation gaps from DFT	BRÜTTING, Moritz
	20	Density Functional Theory (DFT) : Designing Crystalline Piezoelectrics	KUMARI, Geetu
	22	Capturing Solvent Effects in Chromophore Vibrational Spectra DFT-MD Simultations	KEBABSA, Abir
	25	DFT with σ-functionals for highly accurate energies and molecular properties	FAUSER, Steffen
	26	DFT Functionals Simultaneously Targeting Fractional Charge and Spin Challenges	WODYŃSKI, Artur
	36	In situ correction of self-interaction & static correlation errors	BURGESS, Andrew C.
	41	ωB97M-3c: A small basis composite DFT method for the computation of large systems	BÄDORF, Benedikt
	48	Minimal Auxiliary Basis set for TDDFT	DELLA SALA, Fabio
	57	Gauge-problem free local hybrid functionals without calibration function	ARBUZNIKOV, Alexei V.
	75	Understanding ACM performance in the context of density variations	SINGH, Aditi
	86	Regularized second-order energy expressions in context of post-HF and KS-DFT.	SAWICKI, Igor
	87	Representing complicated functionals through neural networks	LOUTIS, Mohamed
	88	One correlation factor to unify them all	ROY, Pierre-Olivier
	101	Hooke's atom: A toy model for DFT	DOMINGUEZ-CALVO, Javier
5. Time-dependent approaches in DFT	19	Developping methods to model excited states in solids: application to minerals	RULLAN, Raphael
	31	Understanding Organic Cocrystals for Room Temperature Phosphorescence	RUEANGBOON, Kanyarat
	40	Density based index based tuning of range-separated hybrid functionals	YAN, Tianhong
	47	in silico design of organic molecules for triplet excited states manipulation	LE BAHERS, Tangui
	63	Exploring natural's dyes color and properties through DFT and TD-DFT	TRAN, Linh Thanh Huyen
	74	Room temperature phosphorescence in matrix-impurity organic crystals	SANDOVAL-SALINAS, Maria Eugenia
	78	RTP coumarin derivatives: TDDFT assessment of the photophysical mechanism	KACZMARCZYK, Dominika
	81	A computational protocol to calculate intersystem crossing rate constants	HE, Yue
	82	Two-photon vibrational spectra of organic dyes: the role of non-Condon couplings	NAIM, Carmelo
	102	A Theoretical Study on Highly Efficient Triplet Harvest in Selone Analogs of PDI	TEDY, Annette
	106	Understanding photophysical features of (metal-)organic systems via TDDFT studies	SREBRO-HOOPER, Monika
	150	A study of the optical properties of a bio-sourced dye	PUSCEDDU, Irene

Poster Session II
Thursday 29th July ; 17:30-20:00

Assigned topic	Subm. ID	Abstract title	Presenter
1. Conceptual DFT	38	The Tilted Plane Condition	BURGESS, Andrew
	117	Elucidating radical C-H functionalization on heteroarenes with a radical GPRI	BARRERA, Yoshio Alan
	159	DFT interpretive tools for describing the effect of microhydration on reactivity	AROULE, Olivier
	170	Fukui function calculation along electronic dynamics simulations	DE LA LANDE, Aurélien
	175	Global/Local Electrophilicity as Measure of Endocrine Disruptor Genotoxicity	JOHNSON, Sophia
	200	Can one hear properties of the molecule?	CHUIKO, Valerii
2. DFT and condensed phases	109	Low-cost computational models of emission processes in supramolecular crystals	HOOPER, James
	112	Ab-initio determination of thermodynamic properties of HNO3-H2O mixtures	LEPRETRE, Julien
	141	A DFT-basedstudyforoptimizingclinoptilolitemodelsandtheircationdistributions	SAEED ABDELRAZIK ALY, Lobna
	152	Effects of inserted methylenes on yields and properties of a molecule transistor	FURUSHIMA, Miku
	161	Hybrid functionals for ABX3 halide perovskites: Influence of Spin-Orbit Coupling	GISSLER, Antoine
	166	DFT calculation for electronic structure of SiC-MOS after NO annealing.	SUGIYAMA, Kosei
	167	DFT study on atomic structures of FeNi/2D materials	MATSUMOTO, Naohiro
	174	New findings on Zintl phased K3Ag3As2 ternary semiconductor compound	MUSEMBI, Robinson
	190	Black Phosphorus and Phosphorene Properties from DFT and TD-DFT	ZHANG, Yu
	191	Modeling the optical properties of biogenic crystals	SENOU, Parfaite
	197	Combined periodic/embedded cluster protocol for modeling adsorption	CURZIETTI, Pietro Maria
	199	DFT investigation of Janus MoSSe/Ga2SSe heterostructures for photocatalysis	YANG, Fan
3. DFT and reactivity	5	Deciphering Regioselective meta-Olefination in Biaryl Systems with DFT Insights	KUMAR, Nikunj
	115	DFT Study of Substituents Effect on Pincer Ligands for CO2 Hydrogenation	GUIMARÃES, Ana
	131	Theoretical Study of Nitrogen Reduction over MXenes	SINGH, Diwakar
	139	Unveiling the OER Mechanism on IrO2(110) – Analysis Beyond Traditional Pathways	USAMA, Muhammad
	140	Assessing the self-polymerization hazards of substances by theoretical chemistry	MACCARONE, Daniele
	142	Early Stages of Diamond Rain formation in Icy Giants.	THEVENET, Thomas
	147	DFT Study of P-Doped Bilayer Graphene Configuration on the ORR in Acidic Solution	LEE, Seung Geol
	148	Electro-oxidation of glucose on n-doped graphene over CrMnFeCoNi HEA	GAKHAD, Pooja
	149	Modeling of Carbonation and Neutralization Reaction for Reinforced Concrete	JEONG, Sohdam
	153	CO2 electrochemical reduction catalyzed by a manganese corrole complex	GARCIA, Gabriela
	157	Bi-Layer Single Atom Catalysts Boosted Nitrate-to-Ammonia Electroreduction	YONG, Xue
	163	Degree of Span Control to Determine the Impact of OER Mechanisms on Co3O4	DHAKA, Kapil
	177	Computational study of pentlandites for the oxygen evolution reaction	SOKOLOV, Maksim
	178	DFT Study of the Steric Effect on Some Methyl Pyridines Adsorption in Zeolite	CASTELLA-VENTURA, Martine
	179	Inter-ionic hydrogen bonds and challenging dimers	MONTERO-CAMPILLO, M Merced
	192	Mechanistic study of a 6-7 switchable acid-catalyzed COT oxide contraction	PEDRÓN, Manuel
	194	g-C3N4/anatase (101) interface for photocatalytic applications: hybrid DFT	WANG, Zihan
4. Methodological Developments in DFT	10	Exploiting the Hessian for a better convergence of the SCF RDMFT procedure	CARTIER, Nicolas
	69	Modern density functionals are ill-designed to compute molecular properties	MATITO, Eduard
	110	Improved Design of Semi-Empirical Density Functional Approximations	PAULAU, Andrei
	111	One-dimensional model for relativistic DFT	AUDINET, Timothee
	137	Ferro and Antiferro couplings in Trinuclear MII-UIV-MII Complexes.	BOUCEKKINE, Abdou
	154	An assessment of XC potentials among hybrid functionals	KUMAR, Vignesh
	160	Dispersion-corrected r^{2}SCAN based double-hybrid functionals	WITTMANN, Lukas
	195	Charge Transfer Imposing Restrictions on the Components of the Dipole Moment	ZÚÑIGA RIVERA, Eduardo
	196	Excited-State Spherical DFT of Coulomb Systems	NAGY, Agnes
	203	Multipole Expansion in Density-Functional Tight-Binding	VUONG, Van-Quan
5. Time-dependent approaches in DFT	113	Benchmarking study of the (X)sTD-DFT methods to compute 1st hyerpolarizabilities	POSTILS RIBÓ, Verònica
	121	Emergence of Localized Surface Plasmon Resonance in Noble Metal Nanoclusters	BRÉMOND, Éric
	127	Tribo-piezoelectric Nanogenerators for Energy Harvesting: first-principles study	DAMTE, Jemal Yimer
	130	Terahertz Laser Pulse Boosts Interlayer Spin Transfer in Heterostructures	LI, min
	145	Resonance-assisted hydrogen bond on 2nd order NLO properties of photoswitches	CHERMETTE, Henry
	162	ESA: Benchmarking Quadratic Response TD-DFT against Higher Levels of Theory	SIRUCEK, Jakub
	189	Electrostatic embedding for excited-state modeling: the case of 2D TMD	HUGUET, Alexandre
	193	DFT based AIMD of a chiral perovskite's spectroscopic properties	ALEHYANE, Amina