The Abdus Salam International Centre for Theoretical Physics

20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods | (SMR 3554)

23 February 2021

Virtual poster session, Italy

1) Methods development

P10	ALVERTIS Antonios Markos	Non-perturbative modelling of exciton-phonon interactions in organic semiconductors
P11	ASIRI Hassn A Yassmin	The harmonic vibrational effects on excitonic gap using QMC and the random thermal averages.
P26	BUSSY Augustin	Efficient and low-scaling linear-response time-dependentdensity functional theory implementation for core-level spectroscopy of large and periodic systems
P27	BUSTAMANTE Carlos Mauricio	A simple approximation to the electron–phonon interaction in population dynamics
P29	CAZZANIGA Marco	Anharmonic calculations of vibrational spectra for molecular adsorbates: A divide-and-conquer semiclassical molecular dynamics approach
P30	CHANEY Gracie	Benchmarking SCAN functional for two-dimensional crystal structures
P32	CHIAROTTI Tommaso	Spectral properties of the interacting homogeneous electron gas from the algorithmic inversion
P40	DE BREUCK Jacques M Pierre-Paul	Machine learning materials properties for small datasets
P75	KO Tsz Wai	A fourth generation high-dimensional neural network potential inclouding non-local charge transfer

2) Energy materials

P02	ACHEHBOUNE Mohamed	Structural, Electronic and optical properties of ZnO doped with Ytterbium (Yb): Overview of DFT calculation
P04	AGBAOYE Ridwan Olamide	Bandgap correction and spin-orbit coupling induced optical absorption spectra of CH3NH2CH3PbI3 for solar cell absorber
P05	AKIODE Kolawole Olubunmi	FIRST PRINCIPLES MODELLING OF SINGLE WALLED CARBON NANOTUBE-METAL OXIDE NANOCOMPOSITE AS ANODE MATERIAL IN LITHIUM ION BATTERY.
P06	ALAM Khorsed	Determining dynamical, mechanical and thermdynamical stability of combinatorially designed ternary transition metal trichalcogenides for potential applications as hydrogen evolution reaction catalysts.
P09	ALLAN Linet	AB-INITIO STRUCTURAL AND ELECTRONIC PROPERTIES OF SELECTED TITANIUM OXIDES AND OXYNITRIDESS
P23	BHAGAT Brajesh Rajesh	Understanding site-dependence overall water splitting mechanism for energetically stable bilayer heptazine g-C3N4
P36	DAS Bikram Kumar	Pure and B/ N doped Graphdiyne as a nano reactor for ORR, a competitor for Platinum: A first principles study

3) Magnetism

P01	ABJAOU Ali	The Magnetic Properties of High Entropy Alloys: Role of Cr on alloy based Al-Fe-Ni-Co
P19	BARBOSA RODRIGUES Joao Nuno	Identifying materials with charge-spin physics from first principles calculations
P21	BELAKROUM Karima	DFT Study of structural, electronic and magnetic properties of CuCrSnS4
P28	CARVALHO Costa Pamela	Investigation of local magnetic properties in metallic multilayered systems
P33	CHIRCHIR Gabriel Kipkemei	INVESTIGATION OF ELECTRONIC, STRUCTURAL AND MECHANICAL PROPERTIES OF FeMnP 1-x A x (A=Si,Ga,Ge ; and) AS A POTENTIAL MAGNETOCALORIC REFRIGERANT ALLOY
P39	DAS Shreya	Understanding the curious magnetic state of Sr3OsO6
P43	DONKOR Edward Danquah	Single-spin Dirac-like states in the rotational graphene phases on Co(0001)
P49	GHOSH Sukanya	Overcoming the asymmetry of the electron and hole doping for magnetic transitions in bilayer CrI3

4) 2D and layered materials

P03	ADANE Tsigie Getie	Electronic Properties of 2D Van der Waals Heterostructures of Janus Transition Metal Dichalcogenides with WS2 Monolayer for Photovoltaic Devices: A First Principle study
P07	ALAM Marwan	First Principles Study of Janus monolaye SnSSe
P12	ATAEI Seyedehsamaneh	Electronic and optical properties of electron-doped layered transition metal dichalcogenides
P13	ATALAR Kemal	Accurate ab initio tight-binding model for twisted bilayer transition metal dichalcogenides
P15	AYARI Sabrine	Phonon-assisted exciton/trion conversion efficiency in transition metal dichalcogenides
P16	BABARIYA Sanjaybhai Bindiya	Tuning the electronic band gap and reflective optical response of 2D layered MoTe2: A DFT study
P24	BŁASZCZAK Jakub Michał	Ab initio' studies of structural and electronic propoerties of orthorombic layered crystals
P25	BONACCI Miki	Excitonic effects in C3N
P31	CHANG Yueqing	z-dependent spin-momentum locking in monolayer 1T'-WTe2
P35	COSTA ALBUQUERQUE Marcelo Fábio	XANESSimulations in Diamond-Like Two-Dimensional Material
P41	DEMIRTAS Merve	Design of two-dimensional ternary Ga2XO structures (X = S, Se, Te)
P42	DIN Haleem Ud	Rashba spin splitting and photocatalytic properties of GeC−MSSe (M=Mo, W) van der Waals heterostructures

5) Surfaces and nanostructures

P14	AYALA Paula María	Ab initio studies of spinel-based γ-Al2O3 surfaces
P97	CEZAR Musseli Henrique	Revisiting greenhouse gases adsorption in carbon nanotubes: advances by ab initio optimized potentials
P45	FOJT Tomasz Jakub	Dipolar coupling of nanoparticle-molecule assemblies: An efficient approach for studying strong coupling
P64	JEYAPRAGASAM Meena Devi	Influence of shape on hydration of gold nanoparticles

6) Molecular and atomic physics

P17	BADRI Ayda	State-to-state inelastic rate coefficients of phosphine in collision with He at low to moderate temperature
P20	BASTOS Alves Vinicius	Beyond-DFT Studies for Thiophene and Furan Oligomers
P54	GUO Jianqing	Hydration of NH + 4 in Water: Bifurcated Hydrogen Bonding Structures and Fast Rotational Dynamics

7) Solid state physics

P08	ALKHALDI Hanof	Computing the Tungsten–Nitrogen Phase Diagram at High Pressure and High Temperature and further ternary W–N compounds
P34	COGOLLO OLIVO Beatriz Helena	Redefining the phase diagram of carbon dioxide within the quasi-harmonic approximation
P38	DA SILVA Lora Estelina	Group Theory Analysis to Study Phase Transitions of Sr3Hf2O7
P50	GOLLAPALLI Prince	Chemically Graded Metal/Ceramic Interface - A High Throughput DFT Study
P52	GORELOV Vitaly	Ab-initio investigation of electronic excitations in bulk V2O5
P55	HASEEN Shariq	Computational structure search of Si3N4
P61	JANIK Norbert	Towards band gap engineering via biaxial and axial strain in group IV crystals
P66	JOSHI Himanshu	Modulation of Optical Absorption in Marcasite Fe1-xRuxS2 and Exploring the Stability of New Phase in RuS2