The Abdus Salam International Centre for Theoretical Physics

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

24 February 2021
Virtual poster session, Italy

1) Methods development

P53	GUANDALINI Alberto	Efficient GW calculations in two dimensional through the interpolation of the screened potential
P56	HEHN Helena Anna-Sophia	Excited-state properties for semi-empirical tight binding
P69	KELLER Levi	Relativistic correction scheme for core-level binding energies from GW
P76	LINSCOTT Edward	Accurately predicting electron affinities with Koopmans spectral functionals
P81	MALICA Cristiano	Temperature-dependent elastic constants from first principles
P89	MIESSEN Alexander	Variational Quantum Algorithms for Real Space Wave Packet Dynamics
P94	MORAES Elizane	Assessment of Density Functionals on Carbon Dioxide intermolecular interactions
P109	PITTS Christopher Thomas	Band-insulators with an odd numbers of electrons per unit cell and a restricted KS method for spin polarised systems
P116	RIEMELMOSER Stefan	RPA-OEP for solids
P117	ROSSMANNEK Max	Quantum HF/DFT-Embedding Algorithms for Electronic Structure Calculations

2) Energy materials

P37	DAS Dr. Tisita	Enhanced Hydrogen Evolution Activity at the Edges of MPSe3 (M= Mn, Fe) Tri-chalcogenide Layers
P44	DUTT Rajeev	Probing of Martensite phase and thermoelectric properties of CoxTaZ(x = 1,2 : Z = Si, Ge, Sn)
P48	GHORUI Supriti	Optoelectronic Properties and Defect Physics of Lead-free Photovoltaic Absorbers Cs2Au(I)Au(III)X6 (X = I, Br)
P73	KOLIOGIORGOS Athanasios	Electronic interaction and energy transfer between Si nanocrystals andorganic chromophores as a function of distance and orientation
P77	LIU Keyang	Ab initio molecular dynamics study of water TiO2 interface
P85	MATERZANINI Giuliana	First-principles discovery of a high-temperature quasi-tetragonal phase in the Li+ conductor Li(3+x)GexP(1-x)O4
P87	MENENDEZ PROUPIN Ariel Eduardo	Atomic scale model and electronic structure of Cu2O/CH3NH3PbI3 interfaces in perovskite solar cells

3) Magnetism

P58	HIDALGO SACOTO Alejandro Raúl	Magnon valley Hall effect in CrI3-based van derWaals heterostructures
P67	JUAN Dilson	Vacancy-driven Magnetic Changes on Doped Manganites: the Effect of a Localized Electronic Defect Level
P79	MAHAJAN Akshay	Decoupled Strain Response of Ferroic Properties in Multiferroic VOCl2 Monolayer
P80	MAHAJAN Ruchika	Self-consistent DFT + U + V study of the structural, electronic, and magnetic properties of Pyrolusite (β − MnO2)
P83	MASROUR Rachid	Electronic, Magnetic properties and magnetocalori ceffect A2BC(A=Fe, Co,..; B=Mn,..; C=Ga, Al,...) Heusler compounds
P90	MIRANDA De Paula Ivan	Ab-initio Gilbert damping on systems with lack of inversion symmetry: Fe50Co50(100) case

4) 2D and layered materials

P47	GARZÓN ARMENDARIZ Nicole Doménica	Bandgap opening in graphene induced by patterned Flower-Like topological defects
P51	GOODWIN Anthony Holmes Zachary	The importance of long-ranged electron-electron interactions on the properties of twisted graphene moiré materials
P57	HERMAN František	Large twisting angles in Bilayer (Moiré) quantum dot structures
P59	JACOBS Rychescki Matheus	Ab initio modelling of laser-induced ultrafast electronic dynamics at the perylene@MoSe2 interface
P60	JAHANGIRZADEH VARJOVI Mirali	Tuning structural and electronic properties of two-dimensional aluminum monochalcogenides: Prediction of Janus Al2XX' (X/X' : O, S, Se, Te) monolayers
P78	MACHEDA Francesco	Theory and Computation of Hall Scattering Factor in Graphene
P92	MISSAOUI Jamil	Role of the valence band on the layer exfoliation in transition metal dichalcogenides: an ab initio study
P100	NERY Juan Pablo	Ab-initio energetics of graphite and multilayer graphene: stability of Bernal versus rhombohedral stacking
P101	NKOU Falonne Bertholde Sharone	Theoretical insights into magnetization in graphene containing single and interacting nanoporous defects
P104	PANDEY Kumar Vineet	Effect of electron-phonon interaction on transprot properties Lead Iodide monolayer
P108	PETERSON Elizabeth	First-principles study of exchange-induced valley splitting in transition metal dichalcogenide monolayers
P113	RAVAL Dharaben Vasantkumar	Ultrahigh carrier mobility and Strain Enhancement properties of 2D penta-PdX2 (X= As, P) monolayer: A DFT study

5) Surfaces and nanostructures

P74	KOTRI Abdelhadi	Static barrier of the clusters on the metallic Cu(111), Ag(111), and Au(111) surfaces
P82	MARSILI Margherita	Combining GW-BSE and PCM approaches for the description of real time electronic dynamics of molecules close to a plasmonic nanoparticle: application to LiCN and p-nitro-aniline (PNA) molecules
P120	SALAZAR MEJÍA Mateo Joshua	Ab-initio studies of ultra-thin CaF2 layers on the Si(100) surface
P122	SANCHEZ NARANJO Anais Jennifer	Computational studies of the electronic structure and stability of TiO2 nanoclusters.

6) Molecular and atomic physics

P62	JAYACHANDRAN Pavithra	Structure and Excitation properties of Functionalized Tin porphyrins: A TDDFT study
P63	JENNIFER G Abigail	Theoretical Insights on the Role of Bis-1,2,3-triazolebipyridine Ligands for Selective Separation of Am(III)/ Eu(III) in Nuclear Waste Management
P65	JIANG Tonghuan	A full configuration interaction quantum Monte Carlo study of transition metal oxide molecules
P84	MASSOTE Daniel Vasconcelos Pazzini	First principles study of atomic boron linear chains with substitutional nitrogen
P93	MONDAL Unmesh	Fundamental studies on the role of nuclear quantum effects in terephthalic acid

7) Solid state physics

P68	KARUNAKARAN Indumathi	DFT STUDY ON GLOBAL REACTIVITY PARAMETERS OF PNA STACKS
P70	KHAEMBA Kennedy Wamalwa	Weyl Chirality in Topological Semimetal Tantalum Phosphide
P72	KOHLI Kanika	Influence of Hydrogen Sulphide and its derivative on the hydrogen permeation through a model PdCu membrane by the first-principles study
P86	MAYDA BACAKSIZ Selma	The degradation of CdS-based paints
P88	MERKEL Ernest Maximilian	CaFeO3 and LaMnO3: octahedral breathing versus Jahn-Teller distortion
P114	REHO Riccardo	Pressure-induced Phase Transitions in Fe4N
P115	REYES LILLO Sebastian Eduardo	First principles calculation of the Hall coefficient in the high-temperature isotropic scattering-time limit
P118	ROSTAMI Samare	Constructing the energy landscape for Ti{x}Zr{1-x}O2 via a neural-network potential through charge equilibration technique