



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

**25 February 2021**  
**Virtual poster session, Italy**

## 1) Methods development

P131	STEIN Frederick	Double-Hybrid DFT Functionals for the Condensed Phase: Gaussian and Plane Waves Implementation and Evaluation
P132	STELLA Martina	Towards a systematic multi-scale method for excitations in molecular materials in the BigDFT code
P167	TANNER Stephen Patrick Daniel	Electrostriction by DFT: a methodological study
P137	TIMROV Iurii	Pulay forces and stresses in density-functional theory with extended Hubbard functionals: From nonorthogonalized to orthogonalized manifolds
P142	TSIRKIN S. Stepan	Enhancing the speed and precision of Wannier interpolation with WannierBerri code
P143	VACONDIO Simone	Higher order many-body perturbation theory applied to atomic systems
P145	VARGAS TELLEZ Alberto Jorge	Improving density functional calculations of molecular polarizabilities using locally scaled self-interaction corrections
P154	WAGNER Kyle Lucas	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians
P156	WHEELER Ashwin William	PyQMC: an all-Python real-space quantum Monte Carlo code
P158	WITT Charles (Chuck) William	Random structure searching with orbital-free density functional theory
P159	WITTEMEIER Nils	Quantum transport with Spin Orbit Coupling

## 2) Energy materials

P91	MISHRA Shashi Bhusan	Reactivity Order Among Low-index Facets of TiO <sub>2</sub> for CO <sub>2</sub> Adsorption and Conversion
P96	MUÑOZ SANTIBURCIO Daniel	Influence of electronic excitations on the formation of defects in GaAs
P98	NAAZ Farha	High throughput computational screening of perovskites for photovoltaics
P105	PARK Heesoo	Cubic Phase Stability of Mixed-cation Perovskites: DFT calculations and machine-learning prediction
P106	PATEL Manushi Jitendra	Ab-initio study of CsPbCl <sub>3</sub> and Mn-doped CsPbCl <sub>3</sub> monolayers as solar cell absorbers
P119	R Sarathkumar	Prediction of Structural, Electronic, Magnetic and Thermoelectric Properties for the InverseHeusler alloy Mn <sub>2</sub> NiSn: A first-principles study
P18	BANERJEE Rudra	Combinatorial search for efficient HER catalyst
P139	T Mohan Aswathi	CO <sub>2</sub> capture, activation and dissociation on the Ti <sub>2</sub> C surface and Ti <sub>2</sub> C MXene: the role of surface structure
P141	TRIVEDI Kumar Ravi	Hydrogen Storage on TM metal doped Mg and ZTC - A density functional investigation
P151	VELANKANNI Nandhakumar	DFT insights into electrocatalytic reduction of CO <sub>2</sub> reduction on PdCu(110) surface

## 3) Magnetism

P21	BELAKROUM Karima	DFT Study of structural, electronic and magnetic properties of CuCrSnS <sub>4</sub>
P102	ODEYEMI Olusanmi Ebenezer	Structural, Electronic, Magnetic and Thermodynamic Properties for XCrGe (X: Hf and Zr) Half-Heusler compounds: First Principle Calculations
P107	PEREIRA CARDOSO Claudia Maria	Electronic and magnetic properties of well defined Gr/Co/Ir(111) and Gr/Fe/Ir(111) heterostructures
P110	PRAKASH Roshme	Half-metallic ferromagnetism in XRuMnGa (X = Co & Ni) quaternary Heusler alloys -DFT study by using generalized gradient approximation (GGA) and modified Becke Johnson (mBJ) methods
P111	PRASAD Babu Baijnath	Tunable spin Hall and spin Nernst effects in Dirac nodal line semimetals XCuYAs (X = Zr, Hf; Y = Si, Ge)
P166	SASANI Ali Resa	magneto electric response in rare earth orthoferrites
P125	SHAPOVALOV Konstantin	Rotopolar coupling driving the antiferroelectric phase transition in PbZrO <sub>3</sub>
P133	TADOUT Mohamed	Effect of the cations distribution on the magnetic properties of SnFe <sub>2</sub> O <sub>4</sub> : First-principles study
P136	THOTTATHIL Reshmi	First Principle Study on Magneto-electric Multiferroics
P162	YADAV Kumar Dinesh	Structural, elastic, electronic, and magnetic properties of MnNbZ (Z = As, Sb) and FeNbZ (Z = Sn, Pb) semi-Heusler alloys
P99	NAMSRAI Tsogbadrakh	First-principles calculation of magnetism and magnetocrystalline anisotropy in antiferromagnetic semiconducting chalcopyrite

#### 4) 2D and layered materials

P07	ALAM Marwan	First Principles Study of Janus monolaye SnSSe
P126	SHARMA Gautam	Structural, electronic and transport properties of Bil 3 /ZrS 2 van der Waals heterostructure: A first principle investigation
P128	SILVA GUILLÉN Jose Angel	Strain tuning of the anisotropy in the optoelectronic properties of the two-dimensional transition metal trichalcogenide TiS3
P130	SPRINGOLO Matteo	Flexoelectricity in two-dimensional materials
P140	TREVIZAM DORINI Thiago	Two-dimensional ABO 3 /Me oxide quasicrystal approximants : insights from Density Functional Theory
P147	VASILCHENKO Vasilii	Polarons In Two-dimensional Pnictogens
P149	VATANKHAHAN Adeleh	Effect of Adsorption of Co and Mn atoms on magnetic and transport properties of hydrogenated borophene nanoribbons
P152	VIPIN KUMAR -	Electric field-induced band modulation of predicted ternary 2D MXC3 [M:X ¼ As:Ge, Sb:Sn and Bi:Pb] with strong stability and optical properties
P153	VITALE Valerio	Chemical trends in the electronic structures of transition metal dichalcogenides
P157	WINES Daniel Thomas	A first-principles Quantum Monte Carlo study of two-dimensional (2D) GaS/Se and Janus GaSSe
P160	WOZNIAK Tomasz	Exciton g-factors of van der Waals heterostructures from first-principles calculations
P163	YUNITASARI Sefty	The study of Dirac cones in graphene flakes using band-unfolding method
P164	ZANOLLI Zeila	Defects in Transition Metal Dichalcogenides: towards quantum computing

#### 5) Surfaces and nanostructures

P123	SANTOS-PUTUNGAN Bernardo Alexandra	Strong chemisorption of CO2 on B10–B13 planar-type clusters
P124	SAPPATI Subrahmanyam	Stability of variable protonation state of citrate on Fe3O4 nanoparticles
P155	WANG Yiyuan	The impact of chemical modification on charge injection at metal/polyolefin interfaces
P165	ZIASHAHABI Azin	Enhanced optical adsorption at the surface of rutile TiO2 nanostructures by oxygen defects

#### 6) Molecular and atomic physics

P103	P Akhileshwari	of intermolecular interaction using Hirshfeld surface analysis and DFT calculations of chalcone derivatives
P46	GARCIA UC Fernando Luis	LDA vs GGA comparative study of the electronic and magnetic properties for dihydrated transition metal oxalate chains
P112	PUGA Anibal Fabian	In Silico prediction of antibacterial activity of sesquiterpene lactones using density-functional theory and quantitative structure-activity relationship methods
P121	SAMBASIVAM Anitha	A DFT Study on the Relationship Between Structure and Antioxidant Properties of Thymoquinone
P138	TISI Davide	Heat transport in water from Deep Neural Network potentials
P144	VAITHIYANATHAN Vetrivelan	Synthesis, Spectral, Hirshfeld surface analysis, DFT calculations and molecular docking studies on dioxol derivatives as potential antibacterial inhibitors

#### 7) Solid state physics

P127	SHEIKH Ali Musharaf	Abinitio Studies on Permeation and Solubility of Hydrogen Isotopes in Iron (Fe), Tungsten (W) and Chromium (Cr)
P129	SONI Gaganbhai Kamalkumar	Compositional dependence of structure and chemical short-range order in Zr-Cu-Al Glass-forming alloys
P134	TAGHIPOUR AZAR Yavar	Termination dependent Rashba-Dresselhaus band splitting in CsPbI3 slabs
P135	TEUNISSEN Leonard Johannes	Automated design of a structural descriptor for radiation resistant perovskites
P146	VÁSCONEZ Marcelo Edwin	First-principles studies of the electronic and mechanical properties of $\alpha$ -Al/ $\gamma$ -Al2O3(111) multilayer composite
P148	VAST Nathalie Madeleine Marguerite	Theoretical phase diagram of boron carbide from ambient to high pressure and high temperature
P150	VEGA David Jorge	Ab Initio study of the structural and electronic properties of Niobium Sulfide (NbS2) and Lithium Niobium Sulfide (LiNbS2) bulk and (001) surfaces
P161	YADAV Kedar	Novel low dense carbon allotropes from data mining approaches