The Abdus Salam International Centre for Theoretical Physics

Workshop on Crystal Structure Prediction: Exploring the Mendeleev Table as a Palette to Design New Materials

14 - 18 January 2019

POSTER SESSION - PRELIMINARY LIST OF POSTER PRESENTATIONS

Presenting author	Poster title
Seyed **AZIMIGEHRAZ**	High-Throughput investigation of close packed Transition Metal surfaces for electrocatalytic reduction of Oxygen
Mohammad Reza **BASAADATKAVKADEHI**	Study of Temperature Effects on Mechanical Properties of Pure Zr and Zr-1%Nb Alloy Using Atomic simulation
El Tayeb **BENTRIA**	Molecular dynamics study of the early stages of metal dusting corrosion on Iron surfaces
Christian **BURNHAM**	A Multipole-Based Crystal Structure Prediction Code
Beatriz **COGOLLO**	Phase diagram of molecular and non-molecular phases of low-Z elements and compounds at extreme pressure and temperature conditions
Grisell **DIAZ LEINES**	Maximum Likelihood Analysis of Reaction Coordinates during Solidification in Ni
Nicholas **FRANCIA**	Towards a computational approach at finite-temperature polymorph screening
Federico **GALLINO**	Crystal Structure Evolution of NiTiCu shape memory alloy
Juan M. **GUERRA**	Ab-initio structural and electronic parameters of thermoelectric $Mg_2X_{1-x}Y_x$ (X,Y=Si,Ge,Sn) alloys
Sebastian **HUTSCH**	The impact of side chain substituents on the morphology of organic crystals
Dilson **JUAN**	Doping Effects on the Migration of Oxygen Vacancies in Lanthanum Strontium Manganite Compound
Qin **KEN**	Difficulty to capture non-additive enhancement of stacking energy by conventional ab-initio methods

Presenting author	Poster title
Rabii **LARHLIMI**	Pressure-induced polimerysazion of CO2 in Li/Na/Mg-Carbon Dioxide phases
Leszek **MALEC**	Ab initio study of polymorphism in urea-barbituric acid co-crystals
Yedilfana S. **MEKONNEN**	Thermodynamic and Kinetic Limitations for Peroxide and Superoxide Formation in Na-O_2 Batteries
Francesca **MENESCARDI**	Towards realistic DFT predictions of materials at high pressure
Sharad **PILLAI**	Strain Effect on Electronic and Lattice Dynamical Behaviour of Two Dimensional Bi BiAs and BiSb
Nawaz **QAISRANI**	On the anomalous photo-physics of single amino acid protein crystals
Seyed Mojtaba **REZAEI SANI**	Theoretical prediction of arsenene for the anode of lithium/sodium-ion batteries: A first-principles study
Samare **ROSTAMI**	Exploring new phases of alkali-halides via a neural-network potential through charge equilibration technique
Pralok **SAMANTA**	Prediction and Ranking of Different Polymorphs of Pharmaceutical Molecules using Basin Hopping Model and Electronic Structure Theory
Raja **SEN**	Understanding the Lithiation of Sn Anode for High-Performance Li-ion Batteries with Exploration of Novel Li-Sn Compounds at Ambient and High Pressure
Arpita **SEN**	TaSi16 clusters on HOPG: structures and electronic properties
Samira **SHEYKHI**	Electronic Structure of UO2 as a Mott Insulator
Mozdeh **SHIRANIRAD**	Accurate and Efficient Calculation of Configurational Contribution to Free Energy of Alloys
Ondrej **TOTH**	Crystal structures of SiOS from evolutionary search up to 100 GPa
Florian **TRYBEL**	Proton dynamics in high-pressure ice-VII from density functional theory
Keishu **UCHIMURA**	Searching for polymer crystals with high thermal conductivities: An ab-initio study
Simon **WENGERT**	Screening Molecular Crystal Structures with Approximate Electronic Structure Methods