The Abdus Salam International Centre for Theoretical Physics

Workshop on Physics and Chemistry of Solid/Liquid Interfaces for Energy Conversion and Storage | (SMR 3577)

24 May 2021 - 28 May 2021
Virtual, Virtual, Italy

P01 - BHATT Bidisha

Dewetting of thin lubricating films under aqueous drops on slippery surfaces

P02 - BISHRUL KAFI Fathima Sheneela

Reduction of chemisorption and surface reactivity of electrodeposited thin film Cu2O/electrolyte junction by surface modification

P03 - BOLARINWA Sherifdeen Oluwaseyi

First-principles insights on the adsorption and gas sensing applications of Bi2O2Se

P04 - COX James Stephen (- not presenting -)

Macroscopic surface charges from microscopic simulations

P05 - DALTON James Stephen

Distributing Nanoparticles Within Materials Can Boost Ionic Conduction, But to What Extent? – A Quantitative Model

P06 - DAS Shyamal Kumar

Rechargeable aqueous aluminum-metal battery: Materials and Challenges

P07 - DEB Jyotirmoy

Twin-graphene: A promissing material for designing of nanoscale capacitor and as an anode material for Na-ion rechargeable batteries

P08 (- not presenting -)

P09 - DE SANTIAGO VARELA Francisco

Lithiation effects on the structural and electronic properties of Si nanowires as a potential anode material

P10 - FACCIO SGIOROVELLO Ricardo Juan

Na and Li-ion titanates for energy applications

P11 - FAYE Omar

Experimental and Theoretical Studies of Hydrogen Generation by Binary Metal (Oxide)-Graphene Oxide Composite Materials

P12 - GIORDANO Livia (- not presenting -)

Reactivity trends at Oxide-Electrolyte Interface in Li-ion Batteries

P13 - GOVINDARAJAN Nitish

Electrolyte effects in electrocatalytic reactions

P14 - HAGOPIAN Arthur

Thermodynamic origin of dendrite growth in metal anode batteries

P15 - JIA Mei (- not presenting -)

Origin of asymmetric electric double layers at electrified oxide/electrolyte interfaces

P16 - JIMENEZ GARCIA Carlos Juan

Effect of Nafion content and hydration level on the electrochemical area of Pt nanocatalyst

P17 - KHALEED Abubakar Abubakar (- not presenting -)

Synthesis of surfactant-free spherical nickel hydroxide/graphene oxide composite for electrochemical capacitor application

P18 - KHOSSOSSI Nabil

Revealing the superlative electrochemical properties of o-B2N2 monolayer in Lithium/Sodium-ion batteries

P19 - KRISTOFFERSEN H Henrik

Towards Constant Potential Modeling of CO-CO Coupling at Liquid Water-Cu(100) Interfaces

P20 - KUMAR Deepak

Metamaterials as Metal – Dielectric Interfaces for Energy Applications

P21 - KUMAR Satendra (- not presenting -)

Alternative for supercapacitors electrode design: Island or fractal-like network

P22 - KUSHWAHA Kumar Anoop

A first principles investigation into halogen-free YBn-1Hn- (Y=C, Si; n=5-14) type anions for high-voltage alkali-metal-ion batteries

P23 - LATIF Hamid

Effect Of SWCNTs Concentration on the Structural Optical and Electrochemical Properties of N-G/Au/SWCNTs Composite

P24 - LIU Sihang

Theoretical Studies of Furfural Electroreduction on Copper Electrode

P25 - LUGINIESKI Marcos

Electrolyte-gated transistor: parameters improvement based on a thin PMMA layer at the electrolyte dielectric/semiconductor interface

P26 - MOHANTY Pankaj

GdCrO4 to GdCrO3 decomposition: Effect of grain interface

P27 - MOHARRAMZADEH GOLIAEI Elham

Recent Developments in Practical Application of TiO2-based Material for Environmental Application

P28 - MONDAL Unmesh

Theoretical investigations of a platinum-water interface using QMM/MM based molecular dynamics

P29 - MULAY R. Manasi

How likely carboxylic acids bind with TiO2 anatase, using Van der Waals corrected DFT methods?

P30 - NEAGU Dragos

Watching nanoparticle exsolution at sub-nanometre, sub-second resolution

P31 - NTIM Samuel

Differential capacitance of ionic liquid confined between metallic interfaces

P32 - OTERO MATO Jose Manuel

Nanoconfined ionic liquids: A computational study

P33 - QAISRANI Muhammad Nawaz

An Ab Intio Molecular Dynamics Study To Investigate The Vibrational Energy Relaxations At Air-Water Interface

P34 - RODRIGUES MIRANDA Caetano

CO selectivity through CO2 hydrogenation at Ni novel catalyst by first principles

P35 - SATAWARA Akshay Mahendrabhai (- not presenting -)

Pd decorated Si2BN nanotube as hydrogen storage candidate: A theoretical insights

P36 - SAVAZZI Filippo

Computational study of reduced Graphene Oxide properties for membrane applications

P37 - SEIDEL Keli Fabiana

Electrolyte-based transistor: improving its efficiency based on electrolyte/semiconductor interface properties

P38 - SHI Haifeng (- not presenting -)

The photoelectrochemical properties of stannum niobate photoanode

P39 - SKACHKOV Dmitry

Atomistic Mechanism of Liquid Ammonia Oxidation on Pt(100) Electrode

P40 - TCHIBOTA POATY Lodvert (- not presenting -)

The oxygen evolution reaction in hematite - Carbon nanotube composites: Insights from density functional theory

P41 - TRYBULA E. Marcela

Atomistic insight into chemistry and properties of pure Al and Al/oxide interface in contact with acidic and alkaline aqueous solutions

P42 - TSALU Vuka Philippe

Interfacial Electronic Effects for Tuning the Chemical Interface Damping

P43 - YILLENG Titus Moses

Synthesis Dependent of Palladium on TiO2 and Their Influences on the Photocatalytic Hydrogen Production from Water