The Abdus Salam International Centre for Theoretical Physics

Workshop on Spectroscopy and Dynamics of Photoinduced Electronic Excitations
8 - 12 May 2017

PRELIMINARY LIST OF POSTER PRESENTATIONS

Presenting author	Poster title
Sara Abass	Structural and Electronic properties of Na2Ti3O7 and H2Ti3O7
Morteza Aghtar	On the origins and an application of two-dimensional hexagonal boron-nitride single-photon emitter
Iorkyaa Ahemen	Spectroscopic investigation of Ce3+/Eu3+ co-doped Li2BaZrO4 nanophosphors
Narjes Ansari	Hole localization in hematite
Sergey Artyukhin	Photoinduced dynamics in IrTe2
Samaneh Ataei	Excitonic effects in the optical properties of hydrogenated TiO2
Rajdeep Banerjee	Identifying optimal dye sensitizers for use in solar cells: DFT studies and descriptors
Victor V. Barsan (Birsan)	New results concerning the generalized Lambert functions and their applications in solar energy conversion
Gabriele Boschetto	Large-scale first principles quantum mechanical calculations on materials for organic photovoltaics
Merabet Boualem	Dual Bi-incorporation effects on optoelectronic properties of CsPbI3 doping MAPbI3 for solar cells
Gloria Capano	Lanthanides Metal Organic Framework (Lns-MOF): Tuning the electronic properties
Ivan Carnimeo	Hartree-Fock exchange calculations with plane waves using localized orbitals
Kevin Conley	TD-DFT calculations of electronic excitations of adsorbed optical dyes at chiral interfaces

Poster sessions 1 & 2 will be held on Wednesday 10 and Thursday 11 May in the Poster Gallery behind the Budinich Lecture Hall. Presenting authors do not need to follow any specific poster board order - no number assigned.

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Diptesh Dey	Quantum dynamics on time-independent and time-dependent PES's
Regiane do Nascimento	Band Gap of BN co-doped Graphene and simulated X-ray absorption spectra, first-principles investigation
Wala Fatheirahman	Quasi-particle and Optical Properties of Hydrogen Titanate
Christine Frayret	Innovation strategies towards the advent of new organic electrodes for energy storage set-ups
Jacopo Fregoni	Azobenzene excited states in the strong coupling regime
Alejandro Gallo Martinez	Ab-initio studies of excited states in vacancy impurity complexes
Kun Gao	Study on the internal conversion dynamics following different electron transfer at a donor/acceptor polymer heterointerface
Fei Gao	Controlling magnetic transition in monovacancy graphene by shear distortion
Samuele Giannini	Computational study of electron and excitation energy transfer in phorphyrin-naphatalenediimide dyads
Mahesh Gudem	Inter system crossing drives the excited hydrogen transfer in ortho Nitrotoluene
Dong Han	Phonon-Enabled Carrier Transport of Localized States at Non-Polar Semiconductor Surfaces: A First-Principles-Based Prediction
Rajeshkumar Hyam	Electron transport and charge transfer dynamics in TiO2 nanostructures for
Mopelola Idowu	Steady and excited state dynamics of lead halide Perovskite Films
Ioana R. Ivascu	Photoacoustic Detection of Pollutant Trace Gases in the Environmental Air
Veljko Jankovic	Origin of Space-separated Charges in Photoexcited Organic Heterojunctions on Ultrafast Time Scales
Joaquim Jornet-Somoza	Exciton dynamics in Light Harvesting Complex-II: From *ab-initio* TDDFT calculations towards Open System models
Ulman Kanchan	Understanding the Electrical Double layer at the Hematite/Water Interface
Khadijeh Khalili	Mapping the charge carrier dynamics in CZTS by time resolved X-ray absorption spectroscopy
Zahra Khatibi	Strain-induced modulation of optical and electronic properties of transition metal dichalcigenides
Shyam Khishor	Dye Sensitized Quantum Dots: First Principles DFT Study
Bernhard Klett	Excitation spectra of molecules within constrained DFT

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Mal-Soon Lee	Structural Rearrangement of Au-Pd Nanoparticles Under Reactions Conditions: An ab Initio Molecular Dynamics Study
Victor Kirui Meng'wa	Structural, Thermodynamic and Electronic properties of Cu2O and CuO nanowires and clusters on TiO2 (101) anatase surface
Alejandro Molina	Ab initio study on the effects of carriers scattering on the optical properties of single-layer transition metal dichalcogenidesî
Juliana M. Morbec	The role of the van der Waals interactions in the absorption of anthracene and pentacene on Ag(111)
Tommaso Morresi	Non adiabatic molecular dynamics: application to graphene syntesis and silica structural relaxation dynamics
Mit H. Naik	Origin of layer dependence in band structures of two-dimensional materials
Zahra Nourbakhsh	Amorphous Matrix Effects on Quantum Confinement in Silicon Nano Slabs
Frank Ortmann	Thermally Activated Charge-Transfer Processes and Polaron Relaxation in Organic Donor-Acceptor Systemsî
Murat Ozkendir	Local Environment Determination of Titanium in Nd(x)Ti(1-x)BO(3) Oxide
Fulvio Paleari	Optical absorption in hexagonal boron nitride multilayers
Javier Pereyra	Photoinduced charge carriers Dynamics on solution-based CuInS2/ZnO Solar cells
PoojaY. Raval	Study on charge transfer in Co_3O_4 by UV-Vis spectral analysis
Fedlu Sabir	Impact of polymer structure on Charge Transport Properties: In connection to grafted side chains
Davide Sangalli	Pump and probe experiments by means of non equilibrium many body green's functions
Filippo Savazzi	An *ab-initio* investigation of the structural deformations and electronic properties of Graphene Oxide
Chhava Sharma	Study of photoinduced electronic excitation/relaxation dynamics using Ultrafast spectroscopy
Haifeng Shi	Photocatalytic reduction of CO2 into Renewable Fuel over C3N4 ,Äìbased composite materials
Michael Walter	Accurate spectroscopy from DFT: from XPS to resonant Raman
Zhi Wang	Ultrafast Charge Transition in CdSe QD/Organic Molecule System: A Real-Time Time-Dependent Ab-Initio Study
Ludger Wirz	Comparison of finite-difference and diagrammatic approaches for the calculation of resonant Raman spectra
Azin Ziashahabi	Study formation mechanism of Zn/ZnO nanoparticles in submerged DC arc discharge by optical emission spectroscopy

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