

18th IASM Poster session (UCD Eng., 13th Jan. 2016, 6 pm)

Queen's University, Belfast

James Cook: Modelling of Magnetic Nanoparticles and their use in Hyperthermic Cancer Treatment

Valerio Rizzi: Electron-phonon thermalisation in real-time quantum dynamics.

Kirsty Whinnery: Molecular Doping on 2D Dichalcogenides : vdW-ab initio calculations

Peter Mulholland: Ionisation and dissociation dynamics of the hydrogen molecular ion and hydrogen molecule

Brian Cunningham: Quasiparticle Self-Consistent GW and the Bethe-Salpeter equation

Dawn Thompson: Nanoparticles for Thermal Energy Storage

Maeve McAllister: Modelling DNA damage caused by Low Energy Electrons

University College Dublin

Aaron Byrne: *Ab-initio* molecular-dynamics study of a dye-sensitised solar cell incorporating a room-temperature ionic liquid as its electrolyte.

Brian Gaynor: DFT-based Mechanistic Determination of Dioxygen Addition to β -diketiminato Ru(II) Complexes

Goar Sánchez-Sanz: Intramolecular Pnictogen Interactions in Naphthalene Derivatives

Trinity College Dublin

Aoife Lucid: The effect of trivalent cation doping on the structure and reducibility of ceria

Aoife Plunkett: The effect of interfaces on the ionic diffusion of F⁻ in CaF₂

Viola Previtali: Probing the phosphates in the ATP molecule with guanidinium systems: a theoretical study

Cristina Trujillo: Understanding the Organocatalytic Asymmetric Reaction Involving Enolizable Anhydrides: A Theoretical Study

Glenn Moynihan: Mechanical Properties of Layered Pnictogen Materials

David O'Regan: Investigation of the Theory of Angular Momentum used in the Quantum-Mechanical Simulation of Magneto- Optical Spectroscopy

Okan Orhan: Towards an accurate optical spectra of bulk gold via first-principles methods

Univ. College Cork and Tyndall Institute

Ekaterina Filatova: Computational Modeling of Atomic Layer Deposition of Silicon Carbide

Ronan Murphy: Reducing the Thermal Conductivity by Driving PbTe to a Phase Transition via Strain and/or Alloying

Marco Fronzi: A first-principles investigation CO₂ interaction with nano-cluster modified TiO₂ rutile(110) and anatase(101) surfaces

Pedram Razavi: Transport in Mesoscopic Systems (TiMeS) on UNICORE

University of Limerick

Sarah Guerin: Molecular modelling of piezoelectricity in biomolecules

Shayon Bhattacharya: Revealing the Extended Structural Geometries of Neurotoxic Proteins: Amyloid Beta and Prion

Pierre-André Cazade: Linkers dynamics in biological nanomachines

Adam Orłowski: How the Carbohydrate-Binding Modules find their way to cellulose

José Luis Domínguez Mejjide: Identification and structural characterisation of the primordial cytotoxic conformers of the amyloidogenic cascade: Preliminary studies

Maynooth Univ.

Matthew Nixon: Molecular recognition and binding mechanisms of XPA by ERCC1 in selected (non-human) species