18th Irish Atomistic Simulators' Meeting, January 2016 (UCD) – Engineering Bldg., room 135

Technical Agenda

Wednesday 13th

11.15-11.45 Coffee and registration

11.50-12.00 Welcome & opening words

Biomolecular Simulation (chaired by Dr. José Angel Martínez-González)

12.00-12.25 Dr. Nicolae-Viorel Buchete
Mapping the kinetic folding network of helical and amyloid-forming peptides

12.25-12.50 Mr. Shane O'Mahony
Modelling protein adsorption on self-assembled monolayer (SAM) surfaces

12.50-1.35 Lunch

1.35-2.00 Ms. Melissabye Gunnoo
Mechanical unfolding of CBM3 domains and its mutants

2.00-2.25 Mr. Colm Herbert
Conformational dynamics and stability of argonaute-2 protein: a molecular-dynamics study

Methodology Development (chaired by Dr. Christian Burnham)

2.30-2.55 Mr. Ryan McMillan
Projected equations-of-motion approach to hybrid quantum/classical dynamics in dielectric-plasmonic composites

2.55-3.20 Dr. Lorenzo Stella
Non-equilibrium molecular dynamics by means of the generalised Langevin equation: theory and a few applications

3.20-3.45 Mr. Douglas Temple
Implementation of a damped dipole-polarisable ionic model within METADISE

3.45-4.10 Tea/coffee

4.10-4.35 Dr. Hender Lopez
Formation of the Nanoparticle Protein Corona: a Coarse-Grained Model

Developments in Irish & European Simulation, and CECAM

4.35-5.45 Discussion and briefing/information session, moderated by Dr. Donal MacKernan

6.00-7.30 Poster Session (third-floor foyer)

Thursday 14th

Materials Simulation (chaired by Drs. Prithwish Nandi & Zdeněk Futera)

9.30-9.55 Mr. Pankaj Kumar
Optical characterisation of native point defects in ZnO

9.55-10.20 Ms. Hayrensa Ablat
Ab initio study of alkyl-cyanoacrylate anionic polymerisation

10.20-10.55 Mr. Conrad Johnston

Investigating nuclear wastes through molecular simulation

11.00-11.30 Tea/coffee

11.30-11.55 Mr. Stephen Osborne
Physisorption of gases into porous liquids

11.55-12.20 Ms. Ailbhe Gavin
Modelling of $LaMnO_3$ for intermediate temperature solid-oxide fuel-cell cathodes

12.20-12.45 Mr. Declan Scullion
Atomic-scale imaging of few-layer black phosphorus and its reconstructed edge: experimental and theoretical approaches

12.50-1.45 Lunch

1.45-2.10 Mr. Michael Ferguson
Understanding Mechanochemical Reactions

2.10-2.35 Dr. Rajarshi Tiwari
Modelling electronic transport in layered organic crystals

2.35-3.00 Ms. Aoife Lucid
Molecular-dynamics investigation of doped ceria materials for solid-oxide fuel-cell electrolytes

3.00-3.30 Tea/coffee

Developments in Molecular Simulation & Industry

3.30-4.00 Discussion session, moderated by Drs. Niall English & Donal MacKernan

4.00-4.10 Closing word

4.15-4.30 Meeting of IASM committee