

NSI MEETING PROGRAMME

12th January

12:00 - 14:00 **Registration - Fitzgerald library**

14:00 - 14:10 **Welcome - SNIAM Lecture Theatre**

Transport I - SNIAM Lecture Theatre

14:10 - 14:30 **A. Hurley**

Spin inelastic transport through magnetic nanostructures

14:30 - 14:50 **S. Bhattacharya**

Charge and spin transport properties of π -conjugated polymers

14:50 - 16:10 **A. Pertsova**

Towards open-boundaries spin-dynamics simulations

16:10 - 16:30 **S. Power** Dynamic RKKY interaction in graphene

16:30 - 17:00 **Coffee Break - Fitzgerald Library**

Surfaces - SNIAM Lecture Theatre

17:00 - 17:20 **M. Nolan**

Engineering TiO_2 interfaces for visible light activated photocatalysis

17:20 - 17:40 **J. Zeglinski** The water-resistant hydroxyl-terminated (010) surface is the dominant surface structure of hydroxyapatite

17:40 - 18:00 **M. Mantega** Hydrogen adsorption configuration and Single Dangling Bond charging state on $\text{Si}(100)\text{-c}(4\times 2)$ for n- and p-type systems

18:00 - 18:20 **C. Patterson** RA and HREELS of Si surfaces

18:45 **Dinner at Fire Restaurant, Dawson Street**

13th January - Parallel Sessions

Transport II - Schrödinger Theatre

09:00 - 09:20 **N. Baadji**

GMR across the phase transition in spin crossover molecules

09:20 - 09:40 **M. Szepieniec** Many-Electron Correlated Scattering: Analytical Approach and Numerical Implementation

09:40 - 10:00 **D. Sharma**

A comparative first-principles approach to the transport properties of Si nanowires

10:00 - 10:20 **T. Archer** Multifunctional tunneling junctions

10:20 - 10:40 **I. Yeriskin** Complex Absorbing Potentials

Techniques - SNIAM Lecture Theatre

09:00 - 09:20 **R. Kováčik** Maximally localized Wannier functions in LaMnO_3 within PBE+ U , hybrid functionals and GW

09:20 - 09:40 **D. MacKernan** Multiscale Dynamical Stochastic Techniques in various Thermodynamics Ensembles and the Adiabatic Approximation

09:40 - 10:00 **M. Shirazi**

Kinetic Monte-Carlo modeling of atomic layer deposition

10:00 - 10:20 **G. Melaugh**

Computer simulation of fluids with intrinsic and permanent cavities

10:40 - 11:40 **Poster Session and Coffee Break - SNIAM Conference**

Materials - Schrödinger Theatre

11:40 - 12:00 **N. M. O'Boyle**

Solving the inverse design problem for polymer solar cells

12:00 - 12:20 **R. Bingham** Self-Organised Lipid Layers on Mercury

12:20 - 12:40 **M. Legesse** First principles study of amorphous, hydrogenated amorphous silicon and interface between crystalline and amorphous silicon

12:40 - 13:00 **A. Narayan**

Andreev Reflection in two-dimensional Topological Insulators

Chemical Physics - SNIAM Lecture Theatre

11:40 - 12:00 **M. Smyth** Excess electron interactions with solvated DNA components: Effect of temperature

12:00 - 12:20 **M. M. El-Hendawy** Evaluation of CO_2 fixation in the cavity of the Rubisco Enzyme using QM, QM/MM and Linear-Scaling DFT methods

12:20 - 12:40 **N. English** Influence of pressure on methane hydrates

12:40 - 13:00 **A. Elena**

Deprotonation mechanism of hydrofluoric acid in $(\text{H}_2\text{O})_7\text{HF}$ cluster

13:00 **Conclusion - Schrödinger Theatre**

LIST OF POSTER TITLES AND FIRST AUTHORS

G. Dey Mechanism of ALD Reaction for Cu

Y. Maimaiti

First Principles Study of Copper Metal ALD from $\text{Cu}(\text{dmap})_2$ and Et_2Zn

S. Klejna First principles modelling of the 'clean-up' effect during atomic layer deposition onto III-V substrates

C. T. Leahy Kinetics of peptide dimer formation

J. Lucid Probing the hydrated phase morphology of hydrated Nafion using temperature-accelerated molecular dynamics simulations

M. Lauricella Study of nucleation mechanism and rate of Methane Hydrate Clathrate

T. Kelly Electron Correlation in Quasi-One-Dimensional Systems: The Emergence of Non-Fermi Liquid Behaviour

S. Meloni Order-disorder phase change in embedded Si nano-particle

R. D. Murphy

Multiscale molecular dynamics study of a helix-turn-helix protein

Z. Hoseyni Exploring the dynamics of AChBP unbound and bound to the Lobeline partial agonist

N. O'Brien

Mechanical behaviour of inter-linked carbon nanotube ropes for nanocomposites