

CMS2017 Meeting Schedule

Sunday 19 March

15.00	Registration opens in the Students Union Building
18.00-21.00	Get together at the Varsity Pub (Adjacent to Main Campus. You can arrive anytime with food served until 9 pm and drinks until later)

Monday 20 March

9.00-9.50	Keynote lecture 1: Prof. Benedetta Mennuci <i>Ab initio simulation of the optical spectroscopy of multichromophoric biosystems</i>
9.50-10.05	Dr. Marco Campetella <i>Ghost states in TDDFT : a reliable descriptor for their detection</i>
10.05-10.20	Prof. Peter Knowles <i>Reaction orbitals: a new paradigm for chemical reaction mechanisms</i>
10.20-11.00	<i>Refreshments</i>
11.00-11.30	Dr. David Benoit <i>Accurate adsorbate vibrations from first principles</i>
11.30-12.20	Keynote Lecture 2: Prof. Todd Martinez <i>Ground and Excited State Dynamics on Graphical Processing Units</i>
12.20-14.00	<i>Lunch</i>
14.00-14.30	Dr. Jonathan Doye <i>Coarse-grained modelling of DNA: From biophysics to nanotechnology</i>
14.30-15.20	Keynote Lecture 3: Prof. Leor Kronik <i>Structure, properties, and spectroscopy of molecular crystals from first principles</i>
15.20-16.00	<i>Refreshments</i>
16.00-16.30	Dr. Gareth Tribello <i>Understanding order-disorder transitions in atomic systems but not quite molecular systems</i>
16.30-16.45	Dr. Stefano Caprasecca <i>Plasmons meet coherences in light-harvesting systems</i>
16.45-17.00	Dr. Marc van der Kamp <i>QM/MM reaction simulation as in silico enzyme activity assay: Applications in antibiotic resistance and biocatalyst evaluation</i>

17.00-17.30	Dr. Andela Saric <i>Amyloid fibrils: formation, self-replication, and inhibition</i>
17.30-17.45	Prof. Michael Bühl <i>Insights into the oxidative power of ligninolytic enzymes from QM/MM calculations</i>
18.30-19.30	<i>Dinner</i>
19.30-22.00	Poster session on Science Concourse

Tuesday 21 March

9.00-9.50	Keynote lecture 4: Prof. Michele Parrinello <i>Entropy as a collective variable</i>
9.50-10.05	Mr. James Dix <i>Nano-scale confinement of water between graphene sheets: how different molecular models affect confined structure</i>
10.05-10.20	Dr. Elise Duboue-Dijon <i>Towards an improved description of ion-protein interactions in MD simulations</i>
10.20-11.00	<i>Refreshments</i>
11.00-11.30	Prof. Syma Khalid <i>Multi-scale simulations of bacterial membranes: successes and outlook for the future</i>
11.30-12.00	Dr. Natalia Martsinovich <i>Computational Design and Computational Characterization of Polymeric Carbon Nitride Photocatalysts</i>
12.00-12.15	Dr. Basile Curchod <i>Towards in Silico Photochemical Experiments with Ab Initio Multiple Spawning</i>
12.15-12.30	Dr. Francesco Ambrosio <i>Electronic structure of the hydrated electron: a hybrid functional study</i>
12.30-14.00	<i>Lunch</i>
14.00-15.00	Keynote Lecture 5: Prof. Daan Frenkel <i>Counting the Uncountable: From Granular Entropy to Materials Science</i>
15.00-15.15	Dr. Timothy Hele <i>Design principles for organic chromophores: creating acenes with intense solar light absorption</i>
15.15-15.30	Dr. Maria Sammalkorpi <i>Molecular modelling as a tool for designing tunable coatings for aqueous dispersion of nanoscale hydrophobic objects</i>

15.30-16.00	<i>Refreshments</i>
16.00-16.15	Prof. Fabio Pietrucci <i>A unified simulation approach to chemical reactions in gas phase and in solution</i>
16.15-16.30	Dr. Adam Kirrander <i>Quantum dynamics and ultrafast X-ray scattering</i>
16.30-17.20	Keynote Lecture 6: Prof. Donald Truhlar <i>Recent Progress in Density Functional Theories</i>
17.20-17.35	Prof. Dmitry Shalashilin <i>New applications of Boxed Molecular Dynamics</i>
19.30	<i>Conference Dinner (Rootes Building)</i>

Wednesday 22 March

9.00-9.30	Dr. Jeremy Richardson <i>Concerted hydrogen-bond breaking by quantum tunnelling</i>
9.30-9.45	Dr. Alex Thom <i>Stochastic Coupled Cluster Theory</i>
9.45-10.00	Mr. Guido Falk von Ruddorf <i>Accelerated hybrid density functional molecular dynamics for the hematite/water interface</i>
10.00-10.30	Dr. James Kermode <i>Multiscale Modelling of Materials Chemomechanics</i>
10.30-11.00	<i>Refreshments</i>
11.00-11.15	Dr. Andriy Vasylenko <i>Encapsulated Nanowires: Boosting Electronic Transport in Carbon Nanotubes</i>
11.15-11.30	Dr. Casper Steinman <i>Embedding with Quantum Drude Oscillators</i>
11.30-11.45	Dr. Linda Zotti <i>Resonant transport and electrostatic effects in single-molecule electrical junctions</i>
11.45-12.35	Keynote Lecture 7: Prof. Gemma Solomon <i>Developing chemical intuition for molecular charge transport</i>