# MM 45: Computational Materials Modelling - Low dimensional systems

Time: Wednesday 17:15–18:30 Location: IFW B

MM 45.1 Wed 17:15 IFW B

**Density functional theory of structural distortion in one dimensional and three dimensional structures** — Uri Argaman, Daniela Kartoon, and •Guy Makov — Dept. of Materials, Ben-Gurion University, Beer-Sheva, Israel

The onset of distortion in one-dimensional monatomic chains with partially filled valence bands is considered to be well established by the Peierls theorem, which associates the distortion with the formation of a band gap and a subsequent gain in energy. Many half-filled p-band materials form complex, semiconducting or semi-metallic crystallographic structures, which are commonly conceived of as distortions of simpler, higher-symmetry structures. Employing modern total energy methods on the test cases of elemental chains and lattices, we reveal that the distortion is not universal but conditional upon the balance between distorting and stabilizing forces. Furthermore, in all systems studied, the electrostatic interactions between the electrons and ions act as the main driving force for distortion, rather than the electron band lowering at the Fermi level as is commonly believed. The main stabilizing force which drives the structures towards their symmetric arrangement is the electronic kinetic energy. Both forces are affected by the external conditions, e.g., stress, and consequently the instability is conditional upon them. These results may shed light on the distortion of more complex structures. Funding Acknowledgement: Support of the Israel Ministry of Science and Technology is acknowledged.

MM 45.2 Wed 17:30 IFW B

**Ab initio study of partial basal dislocations in bilayer graphene and few-layer graphene** — •Pavlos Mouratidis[1], James McHugh[1], Kenny Jolley[1], Malcolm Heggie[1], and Patrick Briddon[2] — [1]Department of Chemistry, Loughborough University, Loughborough, United Kingdom — [2]Newcastle University, School of Engineering, Newcatsle upon Tyne, United Kingdom

Graphite has been the material of choice in construction of nuclear reactors for many years due to its low neutron absorption cross-section and high scattering cross-section. The physical properties of a graphite moderator can greatly influence the cost, safety and lifespan of a reactor. Neutron collision damage in graphite results in the formation of basal dislocations. The subsequent interaction of basal dislocations with each other and the surrounding lattice causes severe dimensional changes along the basal direction.

There has been a lot of interest recently in AB and AC stacking grain boundaries in bilayer graphene. Transition from AB to AC stacking can be described by the glide of partial basal dislocations resulting in expansion of dislocation cores and buckling of the bilayer. Herein we present full ab initio and molecular dynamics calculations of basal dislocation network structures in bilayer graphene and few-layer graphene in large supercells of up to 100 nm.

MM 45.3 Wed 17:45 IFW B

**Continuum modeling of complex solid-state dewetting scenarios by the phase-field method** — •Marco Salvalaglio and Axel Voigt — Institute of Scientific Computing, TU Dresden

Solid-state dewetting is a process through which continuous solid films break and agglomerate to form separated islands. It is a spontaneous phenomenon driven by surface energy minimization, which can occur in thin films via surface diffusion at high temperatures. Although being detrimental during the processing of planar architectures, it may be exploited to obtain a large variety of self-assembled structures in a controlled fashion, such as droplets, nanowires, connected filaments, and pierced films. We present the continuum, phase-field modeling of surface diffusion applied to the study of solid-state dewetting. In particular, the case of monocrystalline films undergoing dewetting on amorphous substrates is addressed, including relevant physical contributions such as surface-energy anisotropy and elasticity effects. The standard approach is discussed, along with recent model improvements. Numerical simulations are shown to reproduce and predict the outcome of annealing experiments for patterned silicon-on-insulator films leading to complex nano-architectures and ultra-long nanowires. Moreover, they assess the role of elasticity in enabling a spinodal solid-state dewetting regime during the annealing of strained thin-crystalline films lying on amorphous substrates.

MM 45.4 Wed 18:00 IFW B

**sp3 Bonded 2-Dimensional Allotrope of Carbon: A First-Principles Prediction** — •Bikram Kumar Das, Dipayan Sen, and Kalyan Kumar Chattopadhyay — Thin Film and Nanoscience Laboratory, Department of Physics, Jadavpur University, Kolkata, India

In this work, using state-of-the-art theoretical calculations, we considered cyclobutane motifs, and investigated whether a sp3 bonded 2-dimensional carbon allotrope could be achieved by assembling ladderane chains. Energetic and dynamic stability studies yielded two such promising structures: one with 4-coordinated carbon atoms, space group PMMA, and a relatively more stable structure with a combination of 3 and 4-coordinated carbon atoms, space group P2/C; both having puckered geometries and partially sp3 C-C bonds. However thermal stability investigations indicated only the lower energy configuration could be stable at ambient temperature and pressure. Electronic structures of the proposed allotropes were studied with density functional theory at rigorous HSE06 level. Investigation of electronic properties of these proposed materials revealed them to be direct-gap semiconductors with small bandgaps. Under in-plane biaxial compressive strains, bandgaps of both were found to decrease; whereas, under similar tensile strains, bandgaps of both were observed to increase up to a strain limit of 5% and 6% for Phase 1 and 2 respectively.The predicted small bandgap values of the proposed allotropes, and especially their convenient tunability is thus highly promising from the perspective of next-generation carbon based microelectronics applications.

MM 45.5 Wed 18:15 IFW B

**Prediction of two-dimensional square-$A_2B$ (A=Cu, Ag, Au, and B=S, Se) auxetic semiconductors with ultra-high negative Poisson*s ratios and unusually low lattice thermal conductivities** — •Xin Chen[1], Duo Wang[1], Xiaobiao Liu[2], Linyang Li[3], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Box 516, 751,20 Uppsala, Sweden — [2]School of Sciences, Henan Agricultural University, Zhengzhou 450002, PR China — [3]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium

Using evolutionary crystal structure search and density functional calculations, we have obtained two-dimensional (2D) structures of $A_2B$ (A=Cu, Ag, Au, and B=S, Se). Structural, electronic and mechanical properties of the global minimum single-layer $A_2B$ structures were studied in detail. These structures have two types of geometries (s(I) and s(II)) with square symmetry, and are named square-$A_2B$ (s-$A_2B$ or s(I/II)-$A_2B$) in this paper. All of the s-$A_2B$ structures are semiconductors with direct bandgaps ranging from 1.09 eV to 2.60 eV. Due to the ionic bonding nature, 2D s-$A_2B$ structures have unusually low lattice thermal conductivities, down to 1.5 Wm*1K*1 at room temperature. Also, s-$A_2B$ structures have ultra-low Young*s moduli, which are lower than most previously reported 2D materials, showing their extraordinary flexibility. Moreover, under the application of strain along the diagonal direction, five of these structuers show in-plane negative Poisson*s ratio (NPR). In particular, the NPR of s(II)-Cu2S can reach up to -1.68, higher than other predicted auxetic materials.