MM 32: Developement of Calculation Methods I

Time: Wednesday 10:15–11:30 Location: C 243

MM 32.1 Wed 10:15 C 243

Insights into Modelling Silica Aerogels: A Computational Approach — •Prakul Pandit[1], Nina Borzecka[1], and Ameya Rege[1,2] — [1]Institute of Materials Research, German Aerospace Center, Cologne, Germany — [2]School of Computer science and Mathematics, Keele University, Staffordshire, England

In recent years, extensive research has focused on comprehending the structure-property relationships of silica aerogels, aiming to tailor their characteristics for specific applications. Several computational studies describing the network formation in these aerogels have been reported, primarily methods based on the Brownian motion of particles. However, these studies simplify the morphology by assuming monodisperse particles and representing the Brownian motion with a singular numerical parameter of particle step size. Additionally, the gelled structure is assumed to represent the final dried structure. In this study, we introduce a model to emulate the gelation kinetics and material behaviour of silica aerogels. Notably, the model incorporates the polydispersity observed in experimental setups, thereby offering a robust depiction of morphology based on experimentally observed condensation kinetics. A pivotal improvement involves correlating model numerical parameters with experimental data to accurately emulate the physical kinetics of the gelation. Furthermore, we utilise finite element methods to analyse the volumetric contraction experienced by the gelled system during and post-drying. Thus, the model aims to present a better computational understanding of silica aerogels, that is both more precise and representative.

MM 32.2 Wed 10:30 C 243

Simulation of properties of anisotropic porous ceramics based on 3D reconstructed microstructures — •Radu Stefan Stirbu[1], Leontin Padurariu[1], Vlad Alexandru Lukacs[1], Fereshteh Falah Chamasemani[2], Roland Brunner[2], and Liliana Mitoseriu[1] — [1]Dielectrics, Ferroelectrics & Multiferroics Group, Faculty of Physics, Alexandru Ioan Cuza University of Iasi, 700506 Iasi, Romania — [2]Department Materials Center, Leoben Forschung GmbH, Leoben A-8700, Austria

The functional properties of electroceramics are strongly dependent on their porosity level, as well as on the microstructural characteristics of the existing pores (size, shape, orientation, distribution, connectivity). In the present work, the dielectric, ferroelectric and piezoelectric properties of porous BaTiO3 ceramics with anisotropic porosity are numerically estimated by using Finite Element Models, with realistic geometrical input, based on X-Ray tomography data. By this method, peculiar features as structural defects, cracks, percolated pores can be locally investigated and their role on the material property failure can be better understood. Further, the dielectric, ferroelectric and piezoelectric properties are estimated and compared to the experimental ones. The employed approach provides a bridge from meso- to macroscale in understanding the relationship between the microstructure and material properties.

MM 32.3 Wed 10:45 C 243

Full anharmonicity of transition states via ab initio machine-learning: Self-diffusion in tungsten — •Blazej Grabowski[1], Xi Zhang[1], and Sergiy Divinski[2] — [1]Institute for Materials Science, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Institute of Materials Physics, University of Münster, 48149 Münster, Germany

We propose an efficient ab initio framework to compute the Gibbs energy of the transition state in vacancy-mediated diffusion including the relevant thermal excitations at density-functional-theory level. With the aid of a bespoke machine-learning interatomic potential, the temperature-dependent vacancy formation and migration Gibbs energies of the prototype system body-centered cubic (BCC) tungsten are shown to be strongly affected by anharmonicity. This finding explains the physical origin of the experimentally observed non-Arrhenius behavior of tungsten self-diffusion. A remarkable agreement between the calculated and experimental curvature of the temperature-dependent self-diffusivity is revealed. The proposed computational framework is robust and broadly applicable, as evidenced by first tests for a hexagonal close-packed (HCP) multicomponent high-entropy alloy. The successful applications underscore the attainability of an accurate ab initio diffusion database.

Zhang, Divinski, and Grabowski, arXiv:2311.00633 (2023).

MM 32.4 Wed 11:00 C 243

Simulation of hot carrier generation and distribution in large plasmonic nanoparticles — •Simão João, Hanwen Jin, and Johannes Lischner — Department of Materials, Imperial College London

Energetic or hot carriers in metallic nanoparticles are generated from the decay of the localized surface plasmon via the Landau damping mechanism and can be harnessed for applications in photocatalysis or sensing. A detailed understanding of hot-carrier properties and their dependence on the nanoparticle size, composition, environment and shape is needed to optimize devices. However, standard electronic structure methods, such as those based on first-principles density-functional theory, cannot be applied to nanoparticles of experimentally relevant sizes. To address this challenge, we use a recently developed approach that combines an atomistic tight-binding description of the nanoparticles with a Chebyshev decomposition of Fermi's golden rule in order to calculate the rate of hot carrier generation and the spatial and energetic distribution of electrons. This opens up the possibility of simulating nanoparticles with millions of atoms. We will present results for gold nanoparticles of different shapes including cubes, octahedra and dodecahedra and discuss their potential for the photocatalytic reduction of CO2 into high-value chemicals.

MM 32.5 Wed 11:15 C 243

Detecting vacancy defects in graphene nanoribbon: a Floquet-Bloch formalism — Gulshan Kumar, Shashikant Kumar, and •Prakash Parida — Department of Physics, Indian Institute of Technology Patna, Bihta, Patna, India

We prescribe a theoretical approach aimed at predicting the spatial position of monovacancy defects within zigzag graphene nanoribbons (ZGNRs) at edges. Our methodology involves a comprehensive study of the Floquet quasi-energy band structure, specifically under the illuminating influence of circularly polarized light. Notably, our findings reveal that the strategic placement of monovacancy defects at edges in ZGNRs possesses remarkable potential in regulating the influential flat band edge state in the quasi-energy spectrum. These fascinating properties and findings can be harnessed and applied for various practical applications, further highlighting the significance and relevance of our theoretical framework.