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LECTURE

"Physicochemical characterization of materials through atomistic and mesoscopic simulations"

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In this seminar, three different applications of atomistic and mesoscopic simulations in the physicochemical characterization of different classes of materials will be presented.

Silicon thin films grown by plasma-enhanced chemical vapor deposition
Plasma-enhanced chemical vapor deposition (PECVD) is a widely used technique for growing thin silicon films for many practical applications in electronics, optoelectronics, and photovoltaics. A detailed kinetic Monte Carlo algorithm has been developed that allows the simulation of the growth of nanocrystalline silicon by PECVD at industrially relevant conditions.[1] Based on a comprehensive set of surface reactions without neglecting important physical mechanisms such as diffusion, the methodology can model PECVD film growth for film thicknesses as large as several hundreds of monolayers.

Polymer melts
Molecular architecture plays a decisive role in the resulting properties of macromolecular materials. Here, examples of how molecular dynamics (equilibrium and non-equilibrium) and dissipative particle dynamics simulations are used to shed light on the molecular mechanisms associated with the complex behavior of cyclic polymer melts [2,3] and amphiphilic polymer co-networks.[4]

Aerosols
Despite recent advances, aerosol transport in the free molecular regime remains poorly understood. Currently, there is an active discussion about the impact of the molecular shape and the detailed interactions between gas molecules [5,6] and small nanoparticles ($d < 10$ nm) on aerosol transport, which are neglected by theoretical approaches and engineering correlations. Here, molecular dynamics (MD) simulations are employed to account for the detailed structure and force fields of gasses and NPs. The simulations reveal that the mean free path of air is 43% smaller than the widely accepted today.[5] The MD-extracted NP diffusivities are used to validate the existing theoretical models in the transition and free-molecular regime. Utilizing the simulation results, a modified Stokes-Cunningham-Millikan expression that can describe the aerosol diffusion from the continuum to the free-molecular regime is derived.[7]

[1] Tsalikis, Baig, Mavrantzas, Amanatides, Mataras, J. Chem. Phys. **139**, 20476 (2013).
[2] Tsalikis, Koukoulas, Mavrantzas, Pasquino, Vlassopoulos, Pyckhout-Hintzem, Wischnewski, Mockenbusch, Richter, Macromolecules **50**, 2565 (2017).
[3] Tsalikis, Mavrantzas, Macromolecules **53**, 803 (2020).
[4] Tsalikis, Ciobanu, Patrickios, Harmandaris, Higuchi, Macromolecules **56**, 9299 (2023).
[5] Tsalikis, Mavrantzas, Pratsinis, Phys. Fluids **35**, 097131 (2023).
[6] Tsalikis, Mavrantzas, Pratsinis, Aerosol Sci. Technol. 2023 (under review).
[7] Karadima, Tsalikis, Mavrantzas, Pratsinis (in preparation).