

"Computational studies of structure formation and dynamic properties of organic molecules at hybrid inorganic/organic interfaces"

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Hybrid structures of organic molecules and inorganic semiconductors combine the favorable properties of each material class into conjugates with great application potential.

The organic parts offer a vast diversity in terms of chemistry and structure.

By manipulating the structure, the optoelectronic properties of the organic parts can be fine-tuned in many subtle ways.

Combined with the influence of inorganic substrates, onto which the organic molecules can be deposited as thin films, Hybrid Inorganic/Organic Structures (HIOS) with well-tailored properties can be created that cannot be realized with either material class alone.

This talk will give an overview of the work in our group to theoretically describe the deposition and thin film growth of organic molecules on inorganic substrates using a multi-scale strategy combining quantum density functional theory, all-atom molecular dynamics and Langevin dynamics simulations, and classical diffusion theory.