INTERNATIONAL SOLVAY INSTITUTES BRUSSELS

SOLVAY COLLOQUIUM

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New avenues in modeling nanoporous materials and their applications at crossroads of quantum mechanics, statistical physics and machine learning

Nanoporous materials are omnipresent in the fields of catalysis, sorption, sensing and crucial for future technologies. Modelling is pivotal to understand the function of nanoporous materials. Ideally it would be possible to design the right material with atomic scale precision for the desired macroscopic function. Modeling realistic functional nanomaterials poses significant challenges. Firstly, nanostructured materials used in applications are far from perfect, they possess a broad range of heterogeneities in space and time extending over several orders of magnitude. Spatial heterogeneities from the subnanometer to the micrometer scale in crystal particles with a finite size and specific morphology, impact the material's dynamics. Secondly, the material's functional behaviour is largely determined by the operating conditions. Currently, there exists a huge length-time scale gap between attainable theoretical length-time scales and experimentally relevant scales.[1-2]

A first important ingredient for modelling nanostructured materials is an accurate representation of the interatomic interactions. Ideally very accurate quantum mechanical methods are used for this purpose. Despite the availability of powerful high-performance computers and the development of advanced methods and algorithms, solving the quantum mechanical many-body problem directly for system sizes comparable to experimental systems remains infeasible.

A second crucial aspect of the modeling exercise is the sampling problem of the multidimensional potential energy surface. Identifying interesting regions in phase space is challenging due to the many degrees of freedom involved. To address this, advanced enhanced sampling methods have been developed, however often these rely on chemical intuition.

Recently new avenues have emerged in modelling nanostructured materials thanks to methodologies integrating concepts from machine learning, quantum mechanics and statistical physics. One notable development is the ability to determine energies and forces using numerical Machine Learning Potentials (MLPs) derived from underlying quantum mechanical data.

To fully integrate MLPs into the catalysis or materials design workflow, it is essential to efficiently generate training data that accurately represent the highly dimensional Free Energy Surface while maintaining chemical accuracy. Addressing this challenge requires methodological advancements that enable the coupling of MLPs with kinetic and sampling models to describe complex dynamical phenomena across a broad range of length and time scales. Within this talk, I will show some of our recent endeavours in this direction.[3-5] As will become clear realistic nanomaterials requires a multidisciplinary vision between physics, chemistry, material science, engineering and machine learning. The methods will be illustrated on timely applications in the fields of heterogeneous catalysis, adsorption and sensing using nanoporous materials.[6]

Monday 12 May 2025 at 4:00 P.M.

COFFEE AND TEA WILL BE SERVED AT 3:45 P.M IN FRONT OF THE SOLVAY ROOM

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