



ParisTech

Chimie ParisTech

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Postdoctoral position with Pr. Alexander Neimark, jointly with the group of Pr. Alain Fuchs at Chimie ParisTech

Molecular simulation and statistical thermodynamics of adsorption deformation of nanoporous materials.

Phenomenon of adsorption-induced deformation attracted recently a considerable attention owing to its relevance to the problems of mechanical stability and integrity of novel nanomaterials. Guest molecules adsorbed in nanopores cause a substantial stress in the host matrix leading to its contraction or swelling and sometimes to morphological transitions. Although various experimental manifestations of adsorption-induced deformation have been known for a long time, a rigorous theoretical description of this phenomenon is lacking. The goal of this project is to devise a rigorous statistical mechanical theory and respective molecular simulation methods for studies of adsorption deformation and mechanical properties of compliant nanoporous materials, such as metal-organic frameworks, pillared clays, and mesoporous molecular sieves. The main challenge is to bridge the theory of elasticity of porous media with and the theory of adsorption and to build a molecular simulation model with prediction capabilities.

Funding. The position offered is part of a collaborative research project “Adsorption-induced deformation of nanoporous materials” led by Profs. Alain Fuchs (Chimie ParisTech) and Alex Neimark (Rutgers University, USA). It is funded through the Blaise Pascal International Chair awarded to A. Neimark. This project offers exceptional opportunities for international collaborations.

The position is for 12 months, and the monthly take-home salary is 1700–1900 € (depending on experience).

Location. Chimie ParisTech is a major French and internationally recognized college of Chemical Engineering, part of the Paris Institute of Technology, with a long tradition in teaching and research excellence. It is located in the center of Paris, at the heart of the “Quartier Latin”, the lively and cultural university district.

Candidates. Applicants should have a PhD in Theoretical/Computational Chemistry/Physics or Chemical Engineering with experience in statistical mechanics and molecular simulation (Monte Carlo simulation, classical density functional theory, theory of elasticity). The position is open starting now.

Application process. Provide your CV, a list of publications, a statement of interest and the names of two referees you worked with, by e-mail to the address below.

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