Università degli Studi di Ferrara

Department of Chemical and Pharmaceutical Sciences

Laboratory of Materials Modeling and Simulations - LMMS

Opening of several positions at the University of Ferrara (UniFe, IT) on the modeling of liquid intrusion in porous materials

Several positions will be opened early next year within the H2020 Future and Emerging Technologies project "**Electro-Intrusion - Simultaneous transformation of ambient heat and undesired vibrations into electricity *via* nanotriboelectrification during non-wetting liquid intrusion-extrusion into-from nanopores**". The theme of the research is investigating the mechanism and energetics of liquid intrusion in porous materials and liquid/solid triboelectrification. The knowledge of these phenomena at the atomistic scale will allow to develop devices to produce electric energy by harvesting vibrational energy produced by human activities (e.g. car shock absorbers) and thermal energy extracted from the environment, which is the final goal of the project.

The successful candidates will develop and apply rare event methods based on classical and/or *ab initio* simulations, including QM/MM approaches. He will contribute to the research and dissemination activities of a consortium involving several European universities, research institutions and industrial partners. Large computational resources are available for the project through the **UniFe** computer facilities as well as **PRACE** resources (already secured).

Responsibilities and tasks

The successful candidate would be responsible for

- Development and application of multi-scale methods for describing the interaction between liquids, possibly solutions, and porous solids;

- Development of suitable rare event approaches for dealing with inertia effects on liquid intrusion/extrusion controlled by free energy barriers;

- Investigation of nanoscale liquid-solid contact electrification;

- Contribute to the development and maintenance of the software required for the implementation of the project;

- Supervision of Master students;

- Pursue collaborations with the partners of the project and other groups within UniFe and in other national and international institutions:

Qualifications

For postdoctoral level positions, candidates should have a PhD degree in theoretical/computational chemistry, physics or related subjects.

The successful postdoc candidate must have a solid knowledge of atomistic or solid-state chemistry/physics, statistical mechanics and experience with classical or *ab initio* simulations. Knowledge of rare event methods will be especially appreciated. Programming experience (e.g. C, C++, Fortran, Python, etc.) is preferred.

Good communication skills in both spoken and written English are a requirement. The ability to work in team, self-motivation and research autonomy are desired skills.

For PhD positions, opening later in the year, candidates should have a Master degree in theoretical/computational chemistry, physics or related subjects.

Further information

For additional information regarding the positions, please contact Dr. S. Meloni (simone.meloni@unife.it).