POST-DOC OPENING: Modeling and molecular simulation of interfaces for a better understanding of (eco)-toxicity

Intro: Applications are welcome for one postdoc position at the Department of Energy (DENERG) of Politecnico di Torino (Turin, Italy - www.polito.it) on modeling and molecular simulation of interfaces for a better understanding of (eco)-toxicity and its implications for energy applications. The fellowship stems from an exciting interdisciplinary research project called NanoInformaTIX ("*Development and Implementation of a Sustainable Modelling Platform for NanoInformatics*", H2020 grant, Grant Agreement number: 814426, http://www.nanoinformatix.eu/), where Politecnico di Torino is the leader of the working group about modelling materials. The goal of NanoInformaTIX is to develop, validate and implement a Sustainable Nanoinformatics Framework (SNF) for the risk assessment of engineered nanomaterials (ENM) about their potential (eco)-toxicity and for informing safer design of quality products. More specifically, the selected candidate for the present position will work with Prof. Pietro Asinari and other members of the multi-Scale ModeLing Laboratory - SMaLL (www.polito.it/small). The fellowship has a duration of one year, and it can be extended up to two years, upon a positive review of the research activities carried at the end of each year.

Requested activities: The successful candidate will focus on:

- performing atomistic simulations of solid/solid and solid/liquid interfaces, including surface chemistry and the interactions with organic matter;

- estimating the potential of mean force (PMF) between two surfaces for investigating adhesion and, in particular, adhesion limits, between nanoparticles and organic matter;

- performing coarse-grained molecular dynamics (CGMD) simulations by validated coarse-grained force fields;

- identifying the overall modelling and simulation architecture, including HPC requirements, MODA datasheets and EU Open Simulation Platforms;

- taking care of all duties expected by the work plan of the NanoInformaTIX project (e.g. interactions with partners, reports, progress meetings, deliverables, etc).

Requested skills: Expertise in heat and mass transfer and applied thermodynamics is mandatory. Proficiency in high-level programming language (e.g. Matlab, Python). Previous experience with molecular dynamics (MD) technique and software is required, and a proved experience with LAMMPS (or GROMACS) will be a plus. Previous experience about computing radial distribution functions (RDFs) and potential of mean forces (PMFs) is required, in order to properly parametrize models for coarse-grained molecular dynamics (GCMD). Good understanding of condensed matter physics and previous experience with high-performing computing (HPC) is highly desirable. Preferential communication language will be English.

How to apply: If the above description matches your expertise and you are dreaming on being part of an international, truly interdisciplinary and vibrant team, we strongly encourage you to apply for this position. Applications (and inquiries) must be sent to Pietro Asinari (e-mail address: pietro.asinari@polito.it), and must include:

1. Academic CV with all relevant scientific publications and experience;

2. 1-page motivation letter;

3. Up to three reference letters.

E-mails must have ***"NanoInformaTIX post-doc position"*** as e-mail subject.