



ParisTech

## École Nationale Supérieure de Chimie de Paris

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www.enscp.fr

### **Postdoctoral position in molecular simulation available at ENSCP (Paris), in the group of prof. Alain Fuchs**

**Molecular simulation of gas coadsorption in novel hybrid materials.** Hybrid organic–inorganic materials, including the topical Metal–Organic Frameworks (MOFs), are widely studied for their remarkable gas storage properties ( $H_2$ ,  $CO_2$ , ...). A global effort is under way to design novel hybrid adsorbents with good  $CO_2$  separation properties and fit for use in industrial conditions.

In this context, we will develop a methodology based on molecular simulation techniques (including, but not limited to, Monte Carlo methods) to reliably predict adsorption and coadsorption properties of novel nitrogen-based hybrid materials, which have been synthesized and characterized by collaborators. Existing intermolecular forcefields will be used and adjusted to better reproduce experimental quantities of interest. We will focus on small gas molecules of particular interest ( $CO_2$ ,  $CO$ ,  $N_2$ ,  $O_2$ ,  $H_2$  and  $CH_4$ ).

To we will also develop and test a non-ideal adsorbed solution theory (NIAST) based on the data obtained by simulation. The NIAST will use simple approximations for the chemical potential of gas and take into account the energetic heterogeneity of adsorbed molecules.

**Funding.** The position offered is part of a collaborative research project “Innovative Materials for  $CO_2$  Capture by Adsorption Technology”. It is funded by the French ANR (*Agence Nationale de la Recherche*, a national funding agency). Part of this project are two academic experimental research groups and R&D engineers from an industrial company, offering great opportunities for experimental–theoretical collaboration. The position is for 12 months, and the monthly take-home salary is 1700–1900 € (depending on experience).

**Location.** The ENSCP is a major French and internationally recognised college of Chemical Engineering, part of ParisTech (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 Physical Chemistry or Materials Science with experience in molecular simulation (molecular dynamics and/or Monte Carlo). 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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