



## Marie Skłodowska Curie Action – Postdoctoral Fellowship 2023 Expression of interest – Hosting offer (MSCA-PF-2023)

Contact Person/Scientist in charge (data of the principal investigator of the research	Dr. Coudert
group/lab or scientific supervisor)  Surname	François-Xavier
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Department /Institute /Centre (data of the centre/department where the fellow would be located	IRCP / Institut de Recherche de Chimie Paris
Address	11 rue Pierre et Marie Curie
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Research Area (Please select the research area: corresponding to the eight MSCA evaluation panels. You can select between one and up to three scientific areas per EOI)	Social Sciences and Humanities (SOC)  Economic Sciences (ECO)  Information Science and Engineering (ENG)  Environment and Geoscience (ENV)  Life Sciences (LIF)  Mathematics (MAT)  Physics (PHY)  Chemistry (CHE)
Brief description of the Centre/Research Group/Team (max. 1,600 characters including spaces: information about the research centre or research group, scientific staff. Please include URL if possible)	The Coudert team is part of the Institut de Recherche de Chimie Paris at PSL University. We are a computational chemistry group, interested in materials science and physical chemistry. We use various methods of theoretical chemistry, including DFT calculations, molecular dynamics, Monte Carlo simulations. We also work with data-based approaches such as high-throughput screening and machine learning.
Project description / Topic of interest (max. 1,800 characters including spaces: short description of the research project / research line where the fellow would be hosted and develop his /her project)	Our research group is centered mainly on molecular simulation at various scales, covering first principles methods (quantum chemistry calculations, ab initio molecular dynamics), classical methods (force field-based molecular dynamics and Monte Carlo), and mesoscopic modeling. Our systems of interest lie in the physical and chemical properties of porous materials, and in particular in the adsorption of fluids and the behavior of nano-confined phases: adsorption in metalorganic frameworks (MOFs), phase transitions, amorphous MOFs, stimuli-responsive frameworks, etc.
Applications: documents to be submitted and deadlines (Please indicate the documents that the candidate fellow should submit to establish contact: CV, letter of motivation, letter of references, etc., please indicate deadline. Recommended deadline: April 2023)	CV, letter of motivation, project proposal.  Deadline: April 2023.