

Post-doctoral position at IFP Energies nouvelles (IFPEN)

Atomic scale modelling of the formation of defects in zeolites and their consequences on acidity

Zeolites are nanoporous materials with well-defined crystalline structures, considered key assets in the on-going transition from fossil to renewable fuels and chemicals. They are crystalline, and their acidity is usually assigned to bridging Si-(OH)-Al groups, which motivated many atomic scale modelling studies. In reality, the picture is far from being so simple, as defects are introduced on purpose in the solid by various post-treatments, to improve its catalytic performance. However, the mechanisms of formation of the defects, beyond point defects, and their consequences on acidity, is poorly understood at the atomic scale.¹ The goal of the current project is to propose relevant models for defects beyond point defects, taking into account the role of the external surface of the crystallites, and quantifying the consequences of these defects on the acidity of the zeolite. Density functional theory calculations will be performed, possibly combined with reactive forcefield calculations, to reach this goal. Acidity estimations will rely on the simulation of the adsorption of probe molecules; combined with the calculation of spectroscopic features. The team has expertise in the simulation of complex zeolitic systems, and in reactive forcefield optimization. This project is part of the CARMEN joint research laboratory (<https://www.lcr-carmen.fr/en>), which guarantees strong interactions with experimental partners, experts in electron microscopy, infra-red spectroscopy and nuclear magnetic resonance.

(1) Chizallet, C., Toward the Atomic Scale Simulation of Intricate Acidic Aluminosilicate Catalysts, *ACS Catal.* **2020**, *10*, 5579-5601.

Main work place : IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, 69360 Solaize, France

Starting date: End 2021 – Beginning 2022

Contract: 12 months, possible extension of 6 extra months.

Gross salary: 3160 euros/month

Applications:

Please contact [Céline Chizallet](mailto:celine.chizallet@ifpen.fr) (IFP Energies nouvelles, Solaize, France) (celine.chizallet@ifpen.fr), and Theodorus de Bruin (IFP Energies nouvelles, Rueil-Malmaison, France) (theodorus.de-bruin@ifpen.fr).

Application documents: CV, motivation letter, two recommendation letters.

About IFP Energies nouvelles

IFP Energies nouvelles is a French public-sector research, innovation and training center. Its mission is to develop efficient, economical, clean and sustainable technologies in the fields of energy, transport and the environment. For more information, see www.ifpen.fr. IFPEN offers a stimulating research environment, with access to first in class laboratory infrastructures and computing facilities.