Subject:
Master degree (M1 / M2): Elucidating catalyst deactivation pathways using molecular dynamics

Contact and supervisors:
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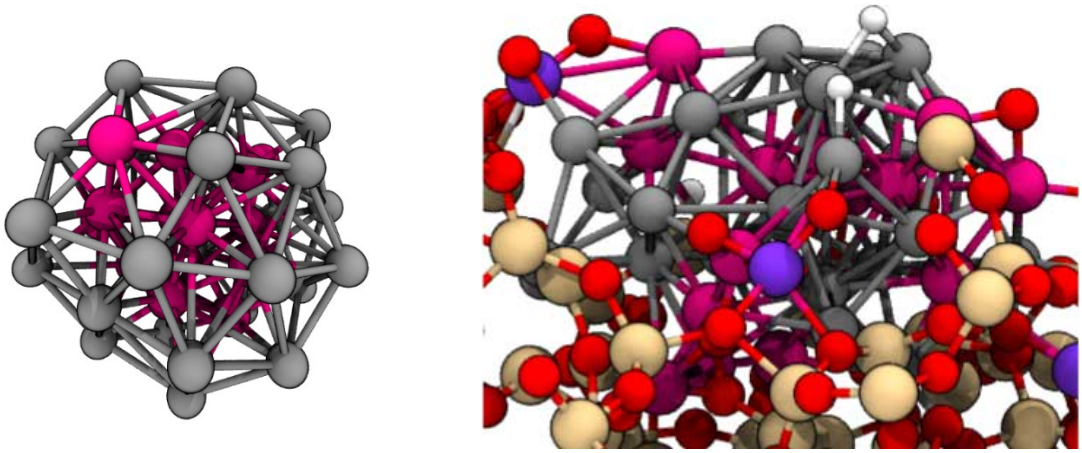
Please send a CV and describe your interest in the research project.

Context:
Major industrial processes rely on heterogeneous catalysts, which consist in metal nanoparticles supported on an oxide (e.g., silica, alumina). **These catalysts are dynamic systems, and reorganize under reaction conditions** due to the presence of reactants and products at elevated temperatures. Some reorganizations are beneficial to the desired activity, while others lead to deactivation, that is the loss of activity and/or selectivity. Owing to the complexity of these systems, they are often poorly understood.

Objective of the internship:
The reorganization of heterogeneous catalysts can involve the whole metal nanoparticle, as well as the oxide support, the reagents and products and even other particles. That is the case for the phenomena **we aim to study: coking, sintering, oxidation, and reduction**. In order to describe these phenomena, we need to rely on realistic models that capture the effect of the different components of a well-characterized system. We've successfully modeled Pt-Ga and Pt-Mn nanoparticles supported on silica to determine their shape and the role of the promoting metal (Ga or Mn).[1]



Reorganization of a Pt-Mn nanoparticle on an amorphous silica support.[1a]

Methods:
To model these complex systems, **the candidate will rely on DFT-level molecular dynamics**, which is capable of describing the electronic structure of the metal, as well as exploring the different configurations of the system. We will also rely on enhanced sampling methods such as metadynamics[2] and blue moon sampling to explore the system more efficiently.

Profile:
The candidate will be able to develop his skills in a broad range of computational techniques, including but not limited to molecular dynamics and metadynamics. **Solid knowledge or previous experience in either molecular dynamics, computational chemistry or heterogeneous catalysis is welcome**, but not mandatory. The candidate will be involved in the design of a research project corresponding to the group's research thematic in heterogeneous catalysis. He or she will as well have opportunities for collaborations with experimental research teams in an international and friendly work environment.

References:
[1] a. L. Rochlitz, Q. Pessemesse, J. W. A. Fischer, D. Klose, A. H. Clark, M. Plodinec, G. Jeschke, P. A. Payard, C. Coperet, *J Am Chem Soc* **2022**, *144*, 13384-13393; b. P. A. Payard, L. Rochlitz, K. Searles, L. Foppa, B. Leuthold, O. V. Safonova, A. Comas-Vives, C. Coperet, *JACS Au* **2021**, *1*, 1445-1458.
[2] G. Bussi, A. Laio, *Nat Rev Phys* **2020**, *2*, 200-212.