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Thomas Pigeon

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Research Experience

Oct 2020 - Oct 2023: **PhD in theoretical chemistry** at IFP Energies nouvelles and INRIA Paris (France)
Combined machine learning and rare event sampling methods to sample reaction trajectories in *ab-initio* molecular dynamics. Work done under the supervision of Pascal Raybaud (IFPEN) and Tony Lelièvre (CERMICS-École des ponts).

Feb 2020 - Aug 2020: **Research internship** at IFP Energies nouvelles (France)
Revisiting edge and surface models for γ-alumina: structural, spectroscopic and reactive properties of sites by DFT calculations (VASP).

Apr 2019 - Aug 2019: **Research internship** in Ayers group at McMaster University (Canada)
Python implementation of a linear response code for linear response and related quantities calculations.

Sep 2018 - Feb 2019: **Research internship** at IFP Energies nouvelles (France)
Building edge models for γ-alumina: structural, spectroscopic and reactive properties of sites by DFT calculations (VASP).

Education

Sep 2019 - Sep 2020: **Master 2: Chemistry, Concepts and Applications** at ENS Lyon (France)
Main courses: Computational chemistry, Quantum approach to catalytic reactivity

Sep 2016 - Sep 2020: **Engineer diploma** at CPE Lyon (France)
Main courses: Theoretical Chemistry, Chemical kinetic, Catalysis, Organic Chemistry

Sep 2014 - Sep 2016: **'Classes préparatoire'** at CPE Lyon (France)
Two years higher education in mathematics, chemistry and physics in preparation for direct entry to CPE Lyon.

Publications

- A.T.F. Batista, T. Pigeon, J. Meyet, D. Wisser, M. Rivallan, D. Gajan, L. Catita, F. Diehl, A-S. Gay, C. Chizallet, A. Lesage, P. Raybaud, Structure, location, and spatial proximities of hydroxyls on γ-alumina crystallites by high-resolution solid-State NMR and DFT modeling: why edges hold the key, ACS Catal. (2023), 6536–6548 (doi:https://doi.org/10.1021/acscatal.3c00495)
- T. Pigeon, C. Chizallet, P. Raybaud. Revisiting γ-Alumina Surface Models through the Topotactic Transformation of Boehmite Surfaces. J. Catal., (2022), 405, (doi:https://doi.org/10.1016/j.jcat.2021.11.011)
- F. Guégan, T. Pigeon, F. De Proft, V. Tognetti, L. Joubert, H. Chermette,P.W. Ayers, D. Luneau, C. Morell, Understanding Chemical Selectivity through Well Selected Excited States, J. Phys. Chem. A, (2020), 124 (doi:10.1021/acs.jpca.9b09978)
- A.T.F. Batista, D. Wisser, T. Pigeon, D. Gajan, F. Diehl, M. Rivallan, L. Catita, A-S. Gay, A. Lesage, C. Chizallet, P. Raybaud, Beyond γ Al_2O_3 crystallite surfaces: The hidden features of edges revealed by solid-state 1H NMR and DFT calculations, J. Catal., (2019), 378, (doi:https://doi.org/10.1016/j.jcat.2019.08.009)

Preprints

- T. Pigeon, G. Stoltz, M. Corral-Valero, A. Anciaux-Sedrakian, M. Moreaud, T. Lelièvre, P. Raybaud, Computing Surface Reaction Rates by Adaptive Multilevel Splitting Combined with Machine Learning and Ab Initio Molecular Dynamics, (arXiv: 2303.05993v1), under reviewing J. Chem. Theory Comput.

Contributions at conferences

Oral presentation

Jan 2023: LIA annual meeting, *Rare event sampling methods and machine learning to study catalytic reaction mechanisms* (slides)

Jan 2023: IFP Énergies nouvelles catalysis, biocatalysis and separation PhD student workshop, *Rare event sampling methods and machine learning to study catalytic reaction mechanisms* (slides)

Feb 2021: ROAD4CAT chair annual meeting, *From boehmite to γ-alumina edges : revisiting the nature of sites and deciphering ^1H NMR experiments* (slides)

Poster presentation

Jan 2023: Mixed-Gen Season 3 – Session 3: Soft matter and machine learning, *Exploring machine learned reaction coordinates in conjunction with rare events sampling methods in ab-initio molecular dynamics for catalytic reactions* (poster)

Oct 2022: Machine Learning Meets Statistical Mechanics: Success and Future Challenges in Biosimulations, *Exploring machine learned reaction coordinates in conjunction with rare events sampling methods in ab-initio molecular dynamics for catalytic reactions* (poster)

Jun 2022: Chasing CVs using Machine Learning: from methods development to biophysical applications, *Exploring machine learned reaction coordinates in conjunction with rare events sampling methods in ab-initio molecular dynamics for catalytic reactions* (poster)

Jun 2022: International Conference on Theoretical Aspects of Catalysis, *Exploring machine learned reaction coordinates in conjunction with rare events sampling methods in ab-initio molecular dynamics for catalytic reactions* (poster)

Mai 2022: Journée plénière GDR IAMAT, *Exploring machine learned reaction coordinates in conjunction with rare events sampling methods in ab-initio molecular dynamics for catalytic reactions* (poster)

Distinctions

Jan 2023: Presentation prize, IFP Énergies nouvelles catalysis, biocatalysis and separation division PhD student Workshop.

Jun 2022: Poster prize, International Conference on Theoretical Aspects of Catalysis

Skills

Programming	Python, basic use of Julia and Fortran
Quantum Chemistry software	VASP, basic knowledge of Orca, Psi4 and Gaussian
Languages	French (native), English (C1 level), German (beginner)
Other	LaTeX, Github, Microsoft Office

PhD Thesis abstract

My thesis work mixes a rare events sampling method (Adaptive Multi-level Splitting, AMS) and machine learning to identify reaction coordinates. The rare events at stake are molecular dynamics transition between identified metastable states (reactant/products). The target is to use machine learning method to define a one dimensional reaction coordinate which will serve to sample reactive trajectories and compute their occurrence probability. The transition mechanism can then be studied by analyzing these trajectories and from their occurrence probability, the reaction rate constant can be computed.
A first part is dedicated to the use of auto-encoders models to define reaction coordinates from a sampling of the Boltzmann-Gibbs measure on two dimensional potentials.
A second part focuses on an iterative approach to learn the committor function using AMS. This last function, mapping the structure coordinates to the probability of reaching first the predefined product state rather that the reactant one, can be considered as an ideal reaction coordinate.
Finally, the last part is dedicated an application to compute reaction rate constants and sample reactive trajectories for a system composed of a catalytic surface on which a water molecule is adsorbed. This application also allows to show how a multiple-state problem can be studied.