Phone: +33 6 58 29 76 95
Lyon, France
thomas.pigeon@cpe.fr

Thomas Pigeon

https://thomaspigeon.github.io
GitHub: thomaspigeon
LinkedIn: thomas-pigeon-b10145155

Work Experience

Oct 2020 - Oct 2023 **PhD in theoretical chemistry** at IFP Energie Nouvelle and INRIA Paris (France)
Combined machine learning and rare event sampling methods to sample reaction trajectories in *ab-initio* molecular dynamics. Machine learning approaches are used to identify collective variables and reaction coordinates that are subsequently used in the adaptive multilevel splitting rare event sampling method to sample reactive trajectories and compute reaction rate constants. This work is done under the supervision of Pascal Raybaud and Tony Lelièvre.

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 (France)
Python implementation of a linear response code for linear response and related quantities calculations.

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

Publications

- 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)

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