Phone: +33 6 58 29 76 95
Lyon
thomas.pigeon@inria.fr

Thomas Pigeon

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

Work Experience

PhD Student **Since Oct 2020**
INRIA and IFP Energie Nouvelles *Paris / Lyon*
PhD in Theoretical Chemistry under the supervision of **T. Lelièvre** and **P. Raybaud**. 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.

Research internship **Feb 2020 - Jul 2020**
IFP Energie Nouvelles *Lyon*
Revisiting edge and surface models for γ-alumina: structural, spectroscopic and reactive properties of sites by DFT calculations(VASP)

Research internship **Apr 2019 - Aug 2020**
Ayers group at McMaster University *Hamilton, Canada*
Python implementation of a linear response code for linear response and related quantities calculations

Research internship **Feb 2020 - Jul 2020**
IFP Energie Nouvelles *Lyon*
Development of γ-alumina edge models by periodic DFT calculations(VASP)

Education

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

Engineer diploma **2016 - 2020**
CPE Lyon
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