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Curriculum Vitae

Thomas Pigeon

July 2021

24 years old
French

RELEVANT EXPERIENCE

- Since Oct 2020 PhD in Theoretical Chemistry under the supervision of **T. Lelièvre** and **P. Raybaud**. Combined machine learned collective variables and rare events sampling method (AMS) to study catalytic reaction mechanisms.
- Feb 2020-Jul 2020: Research internship at **IFP Energies Nouvelles**, Solaize(France) supervisors: **C. Chizallet** and **P. Raybaud**. Revisiting edge and surface models for γ -alumina: structural, spectroscopic and reactive properties of sites by DFT calculations(VASP)
- Apr 2019-Aug 2020: Research internship in **Ayers Group** at **McMaster University**, Hamilton(Canada). Implementation in python of a linear response code for linear response and related quantities calculations
- Sep 2018-Feb 2019: Research internship at **IFP Energies Nouvelles**, Solaize(France) supervisors: **C. Chizallet** and **P. Raybaud**. Development of γ -alumina edge models by periodic DFT calculations(VASP)
- Apr-Jun 2018: 15 days internship at **Institut des Sciences Analytiques**, Lyon(France), supervisor: **C. Morell**. Modifying Fortran codes that determine electronic density polarization to include potential difference perturbations

EDUCATION

- 2019-2020: **ENS Lyon** Master 2: Chemistry, Concepts and Applications
Lessons: Computational chemistry
Quantum approach to catalytic reactivity
- 2016-2020: **CPE Lyon** Graduate school of chemistry and digital science
Graduation expected in November 2020 at MSc level
- 2014-2016: 'Classes préparatoire', two years higher education in mathematics and physics in preparation for direct entry to CPE Lyon

SKILLS

Languages:

- French: Native speaker
English: Operational (C1 level, Cambridge Certificate in Advanced English passed in 2014)
German: Good basic knowledge

Computer skills:

Languages Good basic knowledge of **Python**, and **fortran90**

Quantum chemistry software: Basic knowledge of **ORCA**, **Psi4**, **Gaussian** and **VASP**

PUBLICATIONS

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, 4, 633-641

ATF Batista, D Wisser, T Pigeon, D Gajan, F Diehl, M. Rivallan, L Catita, AS Gay, A Lesage, C Chizallet, P Raybaud, Beyond γ -Al₂O₃ crystallite surfaces: The hidden features of edges revealed by solid-state 1H NMR and DFT calculations - Journal of Catalysis, priority communication 2019, 378, 140-143

INTERESTS AND ACTIVITIES

Play guitar, reading novels