

Paul Clabaut

Academic Experience

Internship and Ph.D. – Since September 2017.....

Title: *Solvation and adsorptions at the solid/water interface: Developments and applications*

Location: *Laboratory of Chemistry, ENS de Lyon, Lyon*

Supervision: MICHEL Carine, STEINMANN Stephan

Description: Development of a computation package to conduct a complex sequence of calculation of free adsorption energies at water/platinum interface. Development and implementation of a force-field for water/metal interactions. AIMD and metadynamics study of alumina hydration.

Short academic collaboration – June/July 2019 (2 months).....

Title: *Collaboration for the elaboration of a Neural-Network based Forcefield*

Location: *UCLA, CA, USA*

Supervision: SAUTET Philippe

Description: Investigation of Machine learning techniques to reproduce metal/water interfacial interactions. Creation of a neural network based on a database of generated interfacial structures.

MSc internship 2 – January to July 2017 (6 months).....

Title: *Elaboration and test of a micro-sized reactor for the plasma-activated catalytic methanation of CO₂*

Location / Supervision: *Institut Pierre-Gilles de Gennes, Paris/ OGNIER Stephanie*

Description: Conception of a micro-sized hybrid plasma/catalyst reactor. Design, work in grey and white room, management and analysis of continuous gaseous flux. M1 student management.

MSc internship 1 – May to July 2016 (12 weeks).....

Title: *Study of alternatives electrochemical techniques of preparation of WO₃ electrodes*

Location / Supervision: *Department of chemistry, University of Michigan, USA / BARTLETT Bart*

Description: Electrodeposition of WO₃ particles on ITO electrodes. Electrochemistry and surface science.

BSc internship – June to July 2015 (8 weeks).....

Title: *Oxygenated heterocycles formation by metal-catalyzed cyclisation*

Location / Supervision: *Laboratory of organic chemistry, ESPCI Paristech, Paris / COSSY Janine*

Description: First laboratory experience. Screening of metal catalysts for an organic chemistry reaction

Scientific communications

Posters.....

Title: *Developing an efficient approach for the computation of solvation free energy at the metal/liquid interface*

Dates: *CP2K day, ENS de Lyon, 02/09/2018 ; SLIMAIA, IFPEN Rueil Malmaison, 03/27-29/2018 ; Journée de la SCF Rhône-Alpes, ENS de Lyon, 06/08/2018; PISACMS summer school, Paris, 08/26/2018 to 09/02/2018; RCTF, Toulouse, 10/8-12/2018, ISTCP, Trömsö, 11-17/07/2019*

Description: Presentation of PhD results about solvation of molecules at the metal/water interface in poster sessions

Oral presentations

Title: *Solvation of noble metals surfaces in water by a local-surface/water forcefield*

Details: *GdR solvate meeting, ENS de Lyon, 3/11/2020*

Description: Presentation of diverse PhD results in a talk session

Title: *Investigating solvation at metal/water interfaces: the SolvHybrid tool fueled by the GAL forcefield*

Details: *JTMS, online, 02/4-5/2019; GdR solvate meeting, online, 25/11/2020*

Description: Presentation of the SolvHybrid and GAL19 articles in a talk session

Published articles

Reactivity of shape-controlled crystals and metadynamics simulations locate the weak spots of alumina in water, *Réocreux, R. and Girel, É. and Clabaut, P. and Tuel, A. and Besson, M. and Chaumonnot, A. and Cabiac, A. and Sautet, P. and Michel, C.*, **Nature Communications**, 2019, doi : 10.1038/s41467-019-10981-9

Water adlayers on noble metal surfaces: Insights from energy decomposition analysis, *Clabaut, P. and Staub, R and Galiana, J. and Antonetti, E. and Steinmann, S.N.*, **The Journal of Chemical Physics**, 2020, 10.1063/5.00130409

Ten Facets, One Force Field: The GAL19 Force Field for Water - Noble Metal Interfaces, *Clabaut, P. and Fleurat-Lessard, P. and Michel, C. and Steinmann, S.N.*, **Journal of Computational and Theoretical Chemistry**, 2020, 10.1021/acs.jctc.0c00091

Solvation Free Energies and Adsorption Energies at the Metal/Water Interface from Hybrid Quantum-Mechanical/Molecular Mechanics Simulations, *Clabaut, P. and Schweitzer, B. and Götz, A. and Michel, C. and Steinmann, S.N.*, **Journal of Computational and Theoretical Chemistry**, 2020, 10.1021/acs.jctc.0c00632

Education

ENS de Lyon & Univerisity Pierre et Marie Curie, Paris

MSc Matter Science & Chemistry

Lyon & Paris

2015–2017

ENS de Lyon

BSc Matter Science & Chemistry (Physics and Chemistry)

Lyon, France

2014–2015

Lycée du Parc

Preparation to french national ranking examination (Chemistry, Physics, and Mathematics)

Lyon, France

2012–2014

Languages

French: Mother tongue

German: Correct mastery

English: Fluent

Japanese: Beginner (A1+)

Informatics skills

Mastered computer languages: Python, latex, bash, awk, fortran90

Mastered utility software: Inkscape, Zotero, Microsoft/Open office

Modelization and theoretical chemistry software: See above

Modelization and theoretical chemistry software

CP2K: Good mastery, code published

ASE: Good mastery

VASP: Correct mastery

AMBER: Correct mastery

Gaussian: Correct mastery

COMSol / Aspen HYSYS: Basic mastery

Organization and responsibility at workplace

Scientific council: Student delegate to the scientific board of the university

PhDday: Organization of a conference day for the PhD students of the lab

Young researcher Seminar: Monthly seminar for the PhD students of the lab (build and organized)

Science days of the ENS: Science popularization for general public

Awards and grants

Study grant: 4 years grant from the French government to study in the ENS

Poster 2nd position award: For the presentation of a poster at PISACMS summer school