

TESSON Stéphane
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EDUCATION

- 2013-2016 Ph.D. - Chemistry-Physics and Analytical Chemistry**
University Pierre et Marie Curie – Paris VI
Laboratory of PHysicochimie des Electrolytes, Nanosystèmes InterfaciaX (PHENIX)
Thesis : A polarizable force field to study clays at the molecular scale
- 2011-2013 Master of Sciences and Technologies in Analytical, Physical and Theoretical Chemistry**
University Pierre et Marie Curie – Paris VI
Received with honors
- 2007-2011 License of Sciences, Technologies and Health in Chemistry**
University Paris Diderot – Paris VII
Received with honors
- 2006-2007 Bachelor of Science – Major: Mathematics**
Montaigne High School, Paris 6th

EXPERIENCES

- 2017 Post-doctoral Researcher** (April 2017 – today) :
Reservoir Engineering Research Institute - Palo Alto & **University of California Riverside** - Riverside (California – United States)
(i) Modelized kerogen systems at the molecular scale.
(ii) Studied the structure of the kerogen systems.
(iii) Studied the dynamics of organic compounds through the kerogen systems.
(iv) Studied the adsorption and desorption phenomena of organic compounds at the kerogen surface.
(v) Scientific mediation: oral communications, writing reports and article.
Supervisors : Prof. Abbas FIROOZABADI & Prof. Jianzhong WU
- 2015 Junior Consultant** (21 months, January 2015 - September 2016)
Materials Design - Montrouge (Île-de-France - France)
(i) Modelized clay minerals at the molecular scale.
(ii) Reviewed the current marketing material on MedeA® capabilities with clay minerals.
(iii) Reviewed and updating the clay minerals structures in MedeA®.
(iv) Developed the automatic assignment parameters of clay minerals in MedeA®.
(v) Tested the implementation of ClayFF and TraPPE in MedeA®.
Supervisors: Ph.D. Philippe UNGERER & Ph.D. Marianna YIANNOURAKOU
- 2013 Ph.D. Candidate** (36 months, October 2013 - September 2016)
PHENIX Laboratory - Paris (Île-de-France - France)
(i) Modelized clay minerals at the molecular scale.
(ii) Parametrized a new model: a polarizable force field.
(iii) Studied the structure of clay minerals.
(iv) Studied the retention, the adsorption and the transport mechanisms of water molecules and ions at the mineral surface.
(v) Scientific mediation: oral and poster communications, writing reports and articles.
Thesis Supervisor: Prof. Virginie MARRY
Secondary supervisors: Ph.D. Benjamin ROTENBERG & Prof. Mathieu SALANNE

Master 2 Internship (6 months, February - August)
LPCM - Sherbrooke (Quebec - Canada)
Atomistic simulation of liquid crystal by molecular dynamics.
Supervisor: Prof. Armand SOLDERA

- 2012** **Master 1 Internship** (5 months, March - July)
CEA/DAM/DIF - Bruyères-le-Châtel (Île-de-France - France)
Simulation of the behavior of rigid molecules under impact by classical molecular dynamics.
Supervisor: Ph.D. Nicolas PINEAU
- 2011** **License 3 Internship** (3 months, April - June)
ITODYS - Paris (Île-de-France - France)
Theoretical study of structural and optical properties of hybrid systems: gold cluster/photochromic molecule.
Supervisor : Ph.D. Aurélie PERRIER
- 2010** **License 2 Internship** (5 months, February - June)
ITODYS - Paris (Île-de-France - France)
(i) *Discovery of the calculation based on quantum chemistry: the study of thermodynamic and optical properties of photochromic molecules.*
(ii) *Studies of spectroscopic properties of different photochromic molecules coupling molecular dynamic/density functional theory.*
Supervisor : Ph.D. Aurélie PERRIER

PUBLICATIONS

- [6] Wu T., Zhao H., **Tesson S.**, Firoozabadi A., *Absolute adsorption and swelling effect of light hydrocarbons and carbon dioxide in shale and isolated kerogen.* (**in prep.**)
- [5] **Tesson S.**, Salanne M., Rotenberg B., Ferrage E., Marry V., *Classical Polarizable Force Field to Study Hydrated Charged Clays and Zeolites: Structure and Dynamics of Ions and Water Molecules.* (**in prep.**)
- [4] **Tesson S.**, Louisfrema W., Salanne M., Anne B., Rotenberg B., Marry V., *Classical Polarizable Force Field to Study Dry Charged Clays and Zeolites.* Journal of Physical Chemistry C, **2017**, 121(18), 9833-9846.
- [3] Porzio F., Cuierrier E., Wespier C., **Tesson S.**, Underhill R. S., Soldera A., *Mechanical Equilibrium, a Prerequisite to unveil auxetic properties in molecular compounds.* Molecular Simulation, **2017**, 43 (3), 169-175.
- [2] **Tesson S.**, Salanne M., Rotenberg B., Tazi S., Marry V., *Classical Polarizable Force Field for Clays: Pyrophyllite and Talc.* Journal of Physical Chemistry C, **2016**, 120 (7), 3749-3758
- [1] Perrier A., **Tesson S.**, Jacquemin D., Maurel F., *On the photochromic properties dithienylethenes grafted on gold clusters.* Computational and Theoretical Chemistry, **2012**, 990 : 167-176.

COMMUNICATIONS (P : POSTER & T : TALK PRESENTATION)

- 2017** Marry V., **Tesson S.**, Louisfrema W., Salanne M., Rotenberg B., Boutin A., Ferrage E., *A classical polarizable force field for the structure and dynamics of water and cations in clays and zeolites,* 16th International Clay Conference (ICC), Granada, Spain, 17-21 July. (**T**)
- 2016** **Tesson S.**, Salanne M., Tazi S., Rotenberg B., Marry V., *Un champ de force polarisable pour étudier la rétention de l'eau et des ions à la surface d'argiles à l'échelle moléculaire,* 14^{ème} colloque du Groupe Français des Argiles (GFA), Poitiers, France, 18-20 May. (**T**)
- Tesson S.**, Salanne M., Tazi S., Rotenberg B., Marry V., *A polarizable force field to study cations and water molecules dynamics in montmorillonites.* 8th International Conference on Porous Media and Annual Meeting, Cincinnati, Ohio, United States, 9-12 May. (**T**)

Tesson S., Salanne M., Tazi S., Rotenberg B., Dubois E., Michot L., Rochet F., Gallet J.-J., Bournel F., Tissot H., Boucly A., Marry V., *Un champ de force polarisable pour étudier la rétention de l'eau et des ions à la surface d'argiles à l'échelle moléculaire*. 5^{èmes} Journées de l'Association Française de l'Adsorption, Paris, France, 4-5 February. (T)

Marry V., **Tesson S.**, Salanne M., Rotenberg B., *Etudes de différentes argiles par dynamiques moléculaire via un champ de force polarisable*. Journée Chimie et Environnement du Labex MiChem, Paris, France, 5 January. (T)

2015 **Tesson S.**, Salanne M., Tazi S., Rotenberg B., Marry V., *Etudes des argiles à l'échelle moléculaire avec un Champ de Force Polarisable*. 16^{ème} Journée Francophones des Jeunes Physico-Chimistes, Playa de Aro-Gérone, Spain, 19-23 October. (T)

Boucly A., Bournel F., Dubois E., Gallet J.-J., Koishi A., Marry V., Michot L., **Tesson S.**, Rochet F., *Etude par NAP-XPS du gonflement d'argiles hectorites et saponites hydroxylées*. 16^{ème} Journée Francophones des Jeunes Physico-Chimistes, Playa de Aro-Gérone, Spain, 19-23 October. (T)

Tesson S., Salanne M., Tazi S., Rotenberg B., Marry V., *Studies of cations and water molecules dynamics in Montmorillonites with a Polarizable Force Field*. Euroclay 2015, Edinburgh, Scotland, 5-10 July. (T)

Tesson S., Salanne M., Tazi S., Rotenberg B., Marry V., *Clays structure and transport in clays with a Polarizable Force Field*. Symposium International MiChem, 2015, Paris, France, 25-26 June. (P)

Boucly A., Bournel F., Dubois E., Gallet J.-J., Koishi A., Marry V., Michot L., **Tesson S.**, Rochet F., *Swelling of hydroxylated hectorite and saponite clays monitored by Near Ambient Pressure-XPS*. Symposium International MiChem, 2015, Paris, France, 25-26 June. (P)

2014 **Tesson S.**, Salanne M., Tazi S., Rotenberg B., Marry V., *Un Champ de Force Polarisable pour les argiles*. Matériaux 2014, Montpellier, France, 24-28 November. (T)

Tesson S., Salanne M., Tazi S., Rotenberg B., Marry V., *Polarizable Force Field for the study of transport in clays at the molecular scale*. 4th Annual NBIA Workshop On ESS Science: Surface Interactions, Copenhagen, Denmark, 10-14 November. (Flash T & P)

Tesson S., Salanne M., Tazi S., Rotenberg B., Marry V., *Champ de Force Polarisable pour l'étude du transport dans les argiles à l'échelle moléculaire*. 24^e Réunion des Sciences de la Terre, Pau, France, 27-31 October. (T)

Tesson S., Salanne M., Tazi S., Rotenberg B., Marry V., *Development of a Polarizable Force Field for clays*. 248th ACS National Meeting & Exposition, San Francisco, CA, United States, 10-14 August. (T invited)

Rotenberg B., Tazi S., Salanne M., Marry V., **Tesson S.**, Sulpizi M., Sprik M., *Interfacial properties of clay minerals : Surface acidity and polarizable force field parametrization from ab-initio simulations*. 247th ACS National Meeting & Exposition, Dallas, TX, United States, 16-20 March. (T)

2013 **Tesson S.**, Porzio F., Soldera A., *Simulation tout atome des phases smectiques C et A d'une famille d'isomères structuraux : 2PhP1, 5PhP1 et 6PhPz*. 16^{ème} Colloque sur les Systèmes Anisotropes Auto-organisés - CFCL13, Collège Doctoral Européen, Strasbourg, France, 3-6 September. (P)

Porzio F., **Tesson S.**, Soldera A., *Peut-on prédire la présence de la phase SmC dans le polymorphisme liquide cristallin d'une molécule?* 16^{ème} Colloque sur les Systèmes Anisotropes Auto-organisés - CFCL13, Collège Doctoral Européen, Strasbourg, France, 3-6 September. (T)

2012 **Perrier A.**, Fihey A., **Tesson S.**, Jacquemin D., Maurel F., *Can photochromic molecules anchored on gold nanoparticles act as nano-hybrid switches?* Second edition of the International Conference on Advanced Materials Modelling (ICAMM), Nantes University, France, 13-16 June. (T)

SKILLS

Computing Operating systems: Windows, Linux and Mac.

Molecular modeling & calculation softwares: Gaussian, LAMMPS, CP2K, Materials Design®, Materials Studio®, GaussView, Molden, Molekel, ChemSketch, VMD and XMakemol.

Programming: C and KSH.

Languages Office automation: MS Office, OpenOffice, Internet (IT and Internet Certificate - Level 1)
French (native) ; English (spoken and written) ; Spanish (notions)

INTERESTS

Music Certificate of Musical Studies (3rd cycle music conservatory)
Licenses Driving license (type B), Boating license (recreational sea waters permit: basic & extended)
Travel Canada, United States and Europe
Sport Table tennis, Badminton and Sail