M. **Simone Pezzotti**
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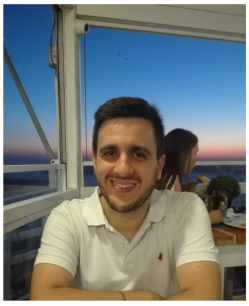

Born on 28 Octobre 1989
Italian nationality

Research interests

I'm specialist in theoretical and computational chemistry for the understanding of physical, spectroscopic and thermodynamic properties of liquid/solid and liquid/vapor interfaces, water in confined environments, and biological interfaces. I like to combine molecular dynamics (ab-initio and classical), theoretical modeling and theoretical vibrational spectroscopy, in synergy with experiments. In particular, I'm interested in hydrophobic effects, their complexity at the molecular scale and their role in biomolecular recognition and phase separation processes in biology. I'm also very interested in hydrophobic hydration at electrochemical interfaces and the multiple roles it plays in catalysis.

Scientific training

2015 - 2019

PhD thesis in physical-chemistry in the group of Prof. Marie-Pierre Gaigeot, Université d'Evry Val d'Essonne & Université Paris Saclay, 20 May 2019. *DFT-MD simulations and theoretical SFG spectroscopy to characterize H-Bonded networks at aqueous interfaces: from hydrophobic to hydrophilic environments.*

May-July 2015

Researcher at LAMBE, UMR 8587, Université d'Evry Val d'Essonne & Université Paris Saclay, in the group of Prof. Marie-Pierre Gaigeot on the theoretical study of the water-air interface.

2009-2015

Bachelor and Master in chemistry at Università di Roma "La Sapienza", specialization in inorganic and physical chemistry (cum laude).

Professional experiences

2021 **Qualification** for associate professor (maître de conférences: sections CNU 28 et 31).

August 2019 - today

Post-Doc researcher in the laboratory "Physical Chemistry II - Laser spectroscopy and Biophotonics", RESOLV, Ruhr University Bochum, in the group of Prof. Martina Havenith on the theoretical quantification and rationalization of solvation entropy contributions in biomolecular processes.

Prices and distinctions

2022 **ERC Starting grant 2022**, for the project ELECTROPHOBIC (PASTEUR, 09/2023).

2019 **Young Investigator Award**, American Physical Society, APS.

2019 **Press interview in the American Institute of Physics (AIP) Publishing**, for the article J. Chem. Phys., 150, 041721 (2019).

Teachings activities

- Co-supervision of students (Bachelor 3 and Master 2) and of PhD students in the group of Prof. Marie-Pierre Gaigeot, Université d'Evry Val d'Essonne & Université Paris Saclay: Debora Beeri, Francesco Amendola, Hermione Decat, Dorian Louaas, Charles Gatine, Fabrizio Creazzo (PhD) et Wanlin Chen (PhD).
- Advanced Practical of Physical Chemistry (laser spectroscopy, RAMAN), Ruhr University Bochum, summer semester 2020 (70h), summer semester 2021 (70h) and summer semester 2022 (70h)
- Label de Chimie Théorique, Réseau Français de Chimie Théorique, January 2020.

Financed research projects

2019

Co-PI of the project "PRACE (Partnership for Advanced Computing in Europe) 18th call". Budget: 33 000 000 h of CPU time on European supercomputers.

2018

Co-PI of the project "PRACE (Partnership for Advanced Computing in Europe) 15th call". Budget: 30 000 000 h of CPU time on European supercomputers.

Administrative activities

- Reviewer for *Journal of American Chemical Society, Molecular Physics, Chemical Reviews, Computational Materials Science, Phys Chem Chem Phys, Nature, Journal of Physical Chemistry, Journal of Chemical Physics.*

Publications

1. S. Pezzotti, F. Sebastiani, E. P van Dam, S. Ramos, V. Conti Nibali, G. Schwaab, M. Havenith. Spectroscopic Fingerprints of Cavity Formation and Solute Insertion as a Measure of Hydration Entropic Loss and Enthalpic Gain. **Angew. Chem., Int. Ed.** 61, e202203893 (2022).
2. M. A. Sani, N. G Pavlopoulos, S. Pezzotti, A. Serva, P. Cignoni, J. Linnemann, M. Salanne, K. Tschulik. Unexpectedly High Capacitance of the Metal Nanoparticle/Water Interface: Molecular-Level Insights into the Electrical Double Layer. **Angew. Chem., Int. Ed.** 134, e202112679 (2022).
3. A. Serva, M. Havenith, S. Pezzotti. The role of hydrophobic hydration in the free energy of chemical reactions at the gold/water interface: Size and position effects. **J. Chem. Phys.** 155, 204706 (2021).
4. C. Y. Ma, S. Pezzotti, G. Schwaab, M. Gebala, D. Herschlag, M. Havenith. Cation enrichment in the ion atmosphere is promoted by local hydration of DNA. **Phys. Chem. Chem. Phys.** 23, 23203(2021).
5. S. R. Alfarano, S. Pezzotti, C. Stein, Z. Lin, S. Funke, K. Mauelshagen, C. Hoberg, C. Y. Ma, T. Ockelmann, G. Schwaab, L. Fu, M. Head-Gordon, M.-P. Gaigeot, K. Tschulik, M. Havenith. Stripping off of the hydration shells in the double layer formation: water networks matter. **Proc. Natl. Acad. Sci.** 118, e2108568118(2021).
6. E. M. Adams, S. Pezzotti, J. Ahlers, M. Ruttermann, M. Levin, A. Goldenzweig, Y. Peleg, S. J. Fleishman, I. Sagi, M. Havenith. Local Mutations Can Serve as a Game Changer for Global Protein Solvent Interaction. **JACS Au** 1, 1076 (2021).
7. S. Pezzotti, A. Serva, F. Sebastiani, F. S. Brigiano, D. R. Galimberti, L. Potier, S. Alfarano, G. Schwaab, M. Havenith, M.-P. Gaigeot. Molecular fingerprints of hydrophobicity at aqueous interfaces from theory and vibrational spectroscopies. **J. Phys. Chem. Lett.** 12, 3827 (2021).
8. A. Serva, M. Salanne, M. Havenith, S. Pezzotti. Size dependence of hydrophobic hydration at electrified gold/water interfaces. **Proc. Natl. Acad. Sci.** 118, e2023867118 (2021).

9. J. Ahlers, E. M. Adams, V. Bader, S. Pezzotti, K. F. Winklhofer, J. Tatzelt, M. Havenith. The key role of solvent in condensation: mapping water in liquid-liquid phase-separated FUS. **Biophys. J.** 120, 1266 (2021).

10. F. Sebastiani, T. A. Bender, S. Pezzotti, W.-L. Li, G. Schwaab, R. G. Bergman, K. N. Raymond, F. D. Toste, T. Head-Gordon, M. Havenith. An Isolated Water Droplet in the Aqueous Solution of a Supramolecular Tetrahedral Cage. **Proc. Natl. Acad. Sci.** 52, 32954 (2020).

11. V. Conti Nibali, S. Pezzotti, F. Sebastiani, D. R. Galimberti, G. Schwaab, M. Heyden, M. P. Gaigeot, M. Havenith. Wrapping Up Hydrophobic Hydration: Locality Matters. **J. Phys. Chem. Lett.** 11, 4809 (2020).

12. O. Kroutil, S. Pezzotti, M.-P. Gaigeot, M. Predota. Phase-Sensitive Vibrational SFG Spectra from Simple Classical Force Field Molecular Dynamics Simulations. **J. Phys. Chem. C.** 124, 15253 (2020).

13. A. Tuladhar, S, Dewan, S. Pezzotti, F. S. Brigiano, F. Creazzo, M.-P. Gaigeot, E. Borguet. Ions Tune Interfacial Water Structure and Modulate Hydrophobic Interactions at Silica Surfaces. **J. Am. Chem. Soc.** 142, 6991 (2020).

14. F. Creazzo, S. Pezzotti, S. Bougueroua, A. Serva, J. Sponer, F. Saija, G. Cassone, M.-P. Gaigeot. Enhanced conductivity of water at the electrified air–water interface: a DFT-MD characterization. **Phys. Chem. Chem. Phys.** 22 (19), 10438 (2020).

15. S. Pezzotti, D. R. Galimberti, M.-P. Gaigeot. Deconvolution of BIL-SFG and DL-SFG spectroscopic signals reveals order/disorder of water at the elusive aqueous silica interface. **Phys. Chem. Chem. Phys.** 21 (40), 22188 (2019).

16. J. D. Cyran, M. A. Donovan, D. Vollmer, F. S. Brigiano, S. Pezzotti D. R. Galimberti, M.-P. Gaigeot, M. Bonn, and E. H. G. Backus. Molecular hydrophobicity at a macroscopically hydrophilic surface. **Proc. Natl. Acad. Sci.** 116, 1520 (2019).

17. F. Creazzo, D. R. Galimberti, S. Pezzotti, M.-P. Gaigeot. DFT-MD of the (110)-Co_3O_4 cobalt oxide semiconductor in contact with liquid water, preliminary chemical and physical insights into the electrochemical environment. **J. Chem. Phys.** 150, 041721 (2019).

18. S. Bougueroua, R. Spezia, S. Pezzotti, S. Vial, F. Quessette, D. Barth, M.-P. Gaigeot. Graph theory for automatic structural recognition in molecular dynamics simulations. **J. Chem. Phys.** 149, 184102 (2018).

19. S. Pezzotti, M.-P. Gaigeot. Spectroscopic BIL-SFG invariance hides the chaotropic effect of protons at the air-water interface. **Atmosphere** 9, 396 (2018).

20. S. Pezzotti, D. Galimberti, Y. Shen, M.-P. Gaigeot. What the diffuse layer (DL) reveals in non-linear SFG spectroscopy. **Minerals** 8, 305 (2018).

21. A. Serva, S. Pezzotti, S. Bougueroua, D. Ruth Galimberti, M.-P. Gaigeot. Combining ab-initio and classical molecular dynamics simulations to unravel the structure of the 2D-HB-network at the air-water interface. **J. Mol. Struct.** 1165, 71 (2018).

22. S. Pezzotti, A. Serva, M.-P. Gaigeot. 2D-HB-Network at the air-water interface: A structural and dynamical characterization by means of ab initio and classical molecular dynamics simulations. **J. Chem. Phys.** 148, 174701 (2018).

23. S. Pezzotti, D. R. Galimberti, Y. R. Shen, M.-P. Gaigeot. Structural definition of the BIL and DL: A new universal methodology to rationalize non-linear $\chi^{(2)}(\omega)$ SFG signals at charged interfaces, including $\chi^{(3)}(\omega)$ contributions. **Phys. Chem. Chem. Phys.** 20, 5190 (2018).

24. S. Pezzotti, D. R. Galimberti, M.-P. Gaigeot. 2D H-bond network as the topmost skin to the air–water interface. **J. Phys. Chem. Lett.** 8, 3133 (2017).

Book chapters

1. S. Bougueroua, V. Chantitch, W. Chen, S. Pezzotti, M.-P. Gaigeot. Direct Dynamics for Vibrational Spectroscopy: From Large Molecules in the Gas Phase to the Condensed Phase. **Vibrational Dynamics Of Molecules**, 416 (2022).

Invited seminars

1. Webinar of the Réseau Français de Chimie Théorique. *Size dependence of hydrophobic hydration at the metal-water interface and its effects on chemical reactions.* 6 May 2021, virtual.

2. Seminar at Institut des Sciences Moléculaires d'Orsay. *Solvation and hydrophobic effects at solid-liquid and biological interfaces from Molecular Dynamics and vibrational spectroscopies.* 19 October 2021, France.

Talks at international conferences

1. WE-Heraeus-Seminar: Entropy and the Second Law of Thermodynamics – The past, the present, and the future. *Mapping local hydration entropy in biology from THz spectroscopy.* 14-17 July 2022, Bad Honnef, Germany.

2. Liquid Matter Conference. *An isolated water droplet in the aqueous solution of a supramolecular tetrahedral cage.* 19-23 July 2021, virtual.

3. 255th ACS National Meeting. *Hydrophobic aqueous interfaces by DFT-MD simulations and vSFG: 2-dimensional H-bond networks.* 18-22 March 2018, New Orleans, USA.

4. CP2K day. (**invited contribution**). *Maximizing water-water interactions at aqueous interfaces: the 2D-Hbond-Network.* 9 February 2018. Lyon, France.

5. Goldschmidt 2017. *SFG Spectroscopy of Silica/water Interfaces by DFT-MD Simulations.* 13-18 August 2017. Paris, France.

6. XXIX IUPAP Conference on Computational Physics, CCP 2017. *SFG Spectroscopy of Silica/water Interfaces by DFT-MD Simulations.* 9-13 July 2017. Paris, France.

Talks at national conferences

1. RESOLV: Summer School Solvation Science 2022. *Adsorption of ions and hydrophobic solutes at electrified interfaces: results from simulations and THz spectroscopy.* 7-9 June 2022, Bochum, Germany.

2. GDR SOLVATE 2022. *Adsorption of ions and hydrophobic solutes at electrified interfaces: results from simulations and THz spectroscopy.* 30-31 May 2022, Paris, France.

3. RESOLV: Spring Workshops. *Size dependence of hydrophobic hydration at electrified gold/water interfaces.* 22-24 March 2021, virtual.

4. RESOLV: Autumn Area Workshops. *Double layer at an electrified interface, beyond the textbook: water matters.* 19 November 2019, Bochum, Germany.

5. JTMS 2019 : Journée Théorie, Modélisation et Simulation. *Horizontal & Vertical ordering at aqueous interfaces.* 5-6 June 2019. Paris, France.

6. Congrès SCF 18. *Maximizing water-water interactions at aqueous interfaces: the 2D-Hbond-Netowrk.* 2-4 July 2018. Montpellier, France.

7. GDR SOLVATE 2018. *Hydrophobic aqueous interfaces by DFT-MD simulations and vSFG: 2-Dimensional H-Bond networks.* 16-17 May 2018. Nancy, France.

8. Journée des Doctorants du LAMBE et DPC. CEA Saclay.*Maximizing water-water interactions at aqueous interfaces: the 2D-Hbond-Network.* 5 December 2017. Paris, France.

9. Journée scientifique de la fédération CPPS Chimie-Physique de Paris-Saclay. *SFG spectroscopy at charged solid/liquid and air/liquid interfaces: new concepts of BIL/DL layers for unraveling spectral signatures.* 20 September 2017. Paris, France.

Poster presentations at conferences

1. SLIMAIA (Solid-Liquid Interfaces: Challenging Molecular Aspects for Industrial Applications). *Air/water and silica/water interfaces characterized by Ab initio Molecular Dynamics.* 27-29 March 2018. Rueil-Malmaison, France.

2. 255th ACS National Meeting. *Air/water and silica/water interfaces characterized by Ab initio Molecular Dynamics.* 18-22 March 2018, New Orleans, USA.

3. 235rd ACS National Meeting. *SFG spectroscopy of silica/water interfaces by DFT-MD simulations.* 2-6 April 2017, San Francisco, USA.

4. DIPC School on Photolectrocatalysis at the atomic scale (PECAS). *Silica/water interfaces structure by DFT-MD simulations.* June 2017, San Sebastien, Spain.

5. Aqueous Interfaces Workshop. *SFG spectroscopy of silica/water interfaces by DFT-MD simulations.* 24 March 2017, Philadelphia, USA.