Stéphane Abel (M)

THE FRENCH ALTERNATIVE ENERGIES AND ATOMIC ENERGY COMMISSION (CEA)
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COMPUTATIONAL CHEMIST AND STRUCTURAL BIOLOGIST

RESEARCH INTEREST

My active research areas include the development of parameters for empirical force fields for simulations of surfactant assemblies (such as membranes, micelles, or inverted micelles). Specifically, I use classical molecular dynamics and quantum simulations to examine interactions between surfactants and membrane peptides/proteins at different atomic levels. I also collaborate in different multidisciplinary projects with various experimental laboratories in France or abroad to study different systems, such as bacterial photosynthetic centers, peptide-peptide interactions (e.g. in the formation of amyloid fibrils), water dynamics around biomolecules or nanomaterials.

PROFESSIONAL SKILLS

- Structural Biology and Chemical Biology (including kinetics, thermodynamics, and quantum chemistry)
- Computer Modeling (Docking) and statistical analysis methods (e.g. Free Energy)
- Programming (Fortran, C++), code development, and software (parallele) architecture
- Teach courses or mentor undergraduates and PhD students

MAJOR EMPLOYMENT EXPERIENCES

THE FRENCH ALTERNATIVE ENERGIES AND ATOMIC ENERGY COMMISSION (CEA) AND THE INSTITUTE FOR INTEGRATIVE BIOLOGY OF THE CELL (I2BC)

08 - Present

Permanent research member in the group “Molecular Simulation of Membrane Systems” CNRS/UMR8821 CEA Saclay (Group leader: Drs. Bruno Robert & M. Marchi).
URL: https://tinyurl.com/yjtm8jzm

LABORATOIRE D’IMAGERIE BIOMEDICAL (FORMERLY LABORATOIRE IMAGERIE PARAMETRIQUE) U. OF PARIS

07 – 08 Post-Doc Fellow in Computational Chemistry in Structural Biology (Supervisors : Dr. Nicolas Taulier)

LABORATOIRE D’IMAGERIE BIOMEDICAL (FORMERLY LABORATOIRE IMAGERIE PARAMETRIQUE) U. OF PARIS

03 – 07 PhD in Molecular Dynamics Simulation in Soft Matter and Structural Biology (Supervisors : Pr. Wladimir Urbach and Dr. Massimo Marchi)

EDUCATION

UNIVERSITY OF PIERRE ET MARIE CURIE (NOW UNIVERSITY OF PARIS) (FRANCE)

03 – 07 PhD fellow In Computational Chemistry in the “Laboratoire d’Imagerie Parametrique” lab CNRS UMR7623. Supervisors: Pr Wladimir Urbach and Dr. Massimo Marchi. (summa cum laude)

AWARDS AND ACHIEVEMENTS

2008: Marie Curie Post-doctoral Fellowship (1 year). 2009: European Biophysical Societies' Association (EBSA) Travel grant.

SCIENTIFIC PRODUCTION

HI = 14; 23 Articles (A) in peer-review journals and 2 Books and Chapters (July 2021)

A1. Baccile N, Seyrig C, Poirier A, Alonso-de Castro S, Roelants SLKW, **Abel S**. 2021 *Self-assembly, interfacial properties, interactions with macromolecules and molecular modelling and simulation of microbial bio-based amphiphiles (biosurfactants). A tutorial review*. *Green Chem.* **23**, 3842–3944. (doi:10.1039/D1GC00097G)

A2. **Abel S**, Marchi M, Solier J, Finet S, Brillet K, Bonneté F. 2021 *Structural insights into the membrane receptor ShuA in DDM micelles and in a model of gram-negative bacteria outer membrane as seen by SAXS and MD simulations*. Biochim. Biophys. Acta - Biomembr. 1863, 183504. (doi:10.1016/j.bbamem.2020.183504)

A3. **Abel S**, Marchi M. 2020 *Deciphering the Structure of the Gramicidin A Channel in the Presence of AOT Reverse Micelles in Pentane Using Molecular Dynamics Simulations*. J. Phys. Chem. B 124, 11802–11818. (doi:10.1021/acs.jpcb.0c08902)

A4. Liang X, Guo C, Liu S, Dang Z, Wei Y, Yi X, **Abel S**. 2018 *Cosolubilization of phenanthrene and pyrene in surfactant micelles: Experimental and atomistic simulations studies*. J. Mol. Liq. 263, 1–9. (doi:10.1016/j.molliq.2018.04.123)

A5. Folpini G, Siebert T, Woerner M, Elsaesser T, **Abel S**, Laage D. 2018 *Librations in Water Nanodroplets Confined in DOPC Reverse Micelles*. In *Conference on Lasers and Electro-Optics*, p. JW2A.120. Washington, D.C.: OSA. (doi:10.1364/CLEO_AT.2018.JW2A.120)

A6. Guettari M, Belaidi A, **Abel S**, Tajouri T. 2017 *Polyvinylpyrrolidone Behavior in Water/Ethanol Mixed Solvents: Comparison of Modeling Predictions with Experimental Results*. J. Solution Chem. 46, 1404–1417. (doi:10.1007/s10953-017-0649-0)

A7. Folpini G, Siebert T, Woerner M, Abel S, Laage D, Elsaesser T. 2017 *Water Librations in the Hydration Shell of Phospholipids*. J. Phys. Chem. Lett. 8, 4492–4497. (doi:10.1021/acs.jpclett.7b01942)

A8. Liang X, Marchi M, Guo C, Dang Z, **Abel S**. 2016 *Atomistic Simulation of Solubilization of Polycyclic Aromatic Hydrocarbons in a Sodium Dodecyl Sulfate Micelle*. Langmuir 32, 3645–3654. (doi:10.1021/acs.langmuir.6b00182)

A9. Karakas E, Taveneau C, Bressanelli S, Marchi M, Robert B, **Abel S**. 2017 *Derivation of original RESP atomic partial charges for MD simulations of the LDAO surfactant with AMBER: applications to a model of micelle and a fragment of the lipid kinase PI4KA*. J. Biomol. Struct. Dyn. 35, 159–181. (doi:10.1080/07391102.2015.1135822)

A10. Djebaili T, **Abel S**, Marchi M, Richardi J. 2017 *Influence of Force-Field Parameters on the Atomistic Simulations of Metallic Surfaces and Nanoparticles*. J. Phys. Chem. C 121, 27758–27765. (doi:10.1021/acs.jpcc.7b09857)

A11. **Abel S**, Galamba N, Karakas E, Marchi M, Thompson WH, Laage D. 2016 *On the Structural and Dynamical Properties of DOPC Reverse Micelles. Langmuir* 32, 10610–10620. (doi:10.1021/acs.langmuir.6b02566)

A12. Djebaili T, Richardi J, **Abel S**, Marchi M. 2015 *Atomistic Simulations of Self-Assembled Monolayers on Octahedral and Cubic Gold Nanocrystals*. J. Phys. Chem. C 119, 21146–21154. (doi:10.1021/acs.jpcc.5b05256)

A13. Marchi M, **Abel S**. 2015 *Modeling the Self-Aggregation of Small AOT Reverse Micelles from First-Principles*. J. Phys. Chem. Lett. 6, 170–174. (doi:10.1021/jz5023619)

A14. Liang X, Zhang M, Guo C, **Abel S**, Yi X, Lu G, Yang C, Dang Z. 2014 *Competitive solubilization of low-molecular-weight polycyclic aromatic hydrocarbons mixtures in single and binary surfactant micelles*. *Chem. Eng. J.* **244**, 522–530. (doi:10.1016/j.cej.2014.01.097)

A15. **Abel S**, Lorieau A, de Foresta B, Dupradeau F-Y, Marchi M. 2014 *Bindings of hMRP1 transmembrane peptides with dodecylphosphocholine and dodecyl-β-d-maltoside micelles: A molecular dynamics simulation study.* Biochim. Biophys. Acta - Biomembr. 1838, 493–509. (doi:10.1016/j.bbamem.2013.10.012)

A16. Djebaili T, Richardi J, **Abel S**, Marchi M. 2013 *Atomistic Simulations of the Surface Coverage of Large Gold Nanocrystals*. J. Phys. Chem. C 117, 17791–17800. (doi:10.1021/jp403442s)

A17. **Abel S**, Dupradeau F-Y, Marchi M. 2012 Molecular Dynamics Simulations of a Characteristic DPC Micelle in Water. J. Chem. Theory Comput. 8, 4610–4623. (doi:10.1021/ct3003207)

A18. **Abel S**, Dupradeau F-YY, Raman EP, MacKerell AD, Marchi M. 2011 Molecular simulations of dodecyl-β-maltoside micelles in water: influence of the headgroup conformation and force field parameters. *J. Phys. Chem. B* **115**, 487–499. (doi:10.1021/jp109545v)

A19. **Abel S**, Waks M, Marchi M. 2010 Molecular dynamics simulations of cytochrome c unfolding in AOT reverse micelles: The first steps. Eur. Phys. J. E 32, 399–409. (doi:10.1140/epje/i2010-10635-x)

A20. **Abel S**, Attia J, Rémita S, Marchi M, Urbach W, Goldmann M. 2009 *Atomistic simulations of spontaneous formation and structural properties of linoleic acid micelles in water*. Chem. Phys. Lett. 481, 124–129. (doi:10.1016/j.cplett.2009.09.033)

A21. **Abel S**, Waks M, Marchi M, Urbach W. 2006 *Effect of surfactant conformation on the structures of small size nonionic reverse micelles: A molecular dynamics simulation study*. Langmuir 22, 9112–9120. (doi:10.1021/la060978v)

A22. **Abel S**, Waks M, Urbach W, Marchi M. 2006 *Structure, Stability, and Hydration of a Polypeptide in AOT Reverse Micelles*. J. Am. Chem. Soc. 128, 382–383. (doi:10.1021/ja053043u)

A23. **Abel S**, Sterpone F, Bandyopadhyay S, Marchi M. 2004 *Molecular Modeling and Simulations of AOT–Water Reverse Micelles in Isooctane: Structural and Dynamic Properties*. J. Phys. Chem. B 108, 19458–19466. (doi:10.1021/jp047138e)

C1. **Abel S**. and Waks M.. "Computational Methods as Tools for the Study of Reverse Micelles Structures and Dynamics: Effect on Confined Biomolecules". In book: Micelles: Structural Biochemistry, Formation and Functions & Usage. Publisher: Nova Science Pub Inc, Editors: Danielle Bradburn, Tom Bittinger, pp. 73-126 ISBN: 978-1629484440

B1. **Abel S.** Micelles inverses d'AOT et de C12E4 "Structure et évaluation de leurs compressibilités par simulation de dynamique moléculaire" (2010); Publisher: EUE, ISBN: 6131533792 (In French)

REVIEWING AND EVALUATION

Regular referee (~7 papers/year) for academic journals (*e.g. JPCB, Langmuir, JCTC, Molecular Simulation*) Grant evaluations for French universities and European Organizations (PRACE).

TEACHING AND SUPERVISION RESPONSIBILITIES	Participate actively in the teaching of Biophysics, Biochemistry and Molecular Simulations (mostly for 2nd and 3rd year students). I also supervise students for their research Master and PhD projects.
PROFESSIONAL AND SCIENTIFIC ORGANIZATION	Member of the American Biophysical Society and the French Biophysical Society (2007-present).