

Curriculum Vitae

Stéphane Abel

DOB: October, 9, 1973

Paris, France

**Researcher in Computational Chemistry and Biochemistry
and Permanent Member in the laboratory
« Molecular simulation of membrane systems »
CNRS/UMR8821
Commissariat à l'énergie atomique et aux énergies alternatives
(CEA)**

Personal address:

6 Impasse Baudran

F-75013, Paris, France

Telephone: +33 6 49 37 70 60

Web : <http://www.st-abel.com>

Professional address:

CEA Saclay, DSV/iBiTec-S/SB2SM/LBMS

& CNRS UMR8821

F-91191 Gif-sur-Yvette, Cedex, France

Telephone: +33 1 69 08 72 92

Mail : stephane.abel@cea.fr

https://www.researchgate.net/profile/Stephane_Abel/

Education

92 - 98 Natural Sciences in structural biology, biochemistry, University of Bordeaux and Pierre and Marie Curie (Fr) (Bsc.)

99 - 02 Computer sciences of Pierre and Marie Curie and Rennes I universities (Fr).

03 - 07 Ph.D. Student in Computational Chemistry in the "Laboratoire d'Imagerie Paramétrique" CNRS UMR7623. Supervision: Dr Wladimir Urbach and Massimo Marchi. (*summa cum laude*)

Major Employment Experiences

08 to Present Permanent research member in the group "Molecular Simulation of Membrane Systems" CNRS/UMR8821 CEA Saclay (leader: Dr. M. Marchi).

07 - 08 Post-doctoral research "Molecular simulation of membrane systems"

03 - 07 Ph.D. student (4 years) in the "Laboratoire d'Imagerie Paramétrique" UMR7623 (Laboratory of Dr. P. Laugier).

Awards and Achievements

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

Research Interests

My active areas of research include the development of parameters for empirical force fields for simulations of surfactant assemblies (such as membrane, micelles or reverse micelles). More specifically, I use various computational methods that combine Molecular Dynamics

and Quantum Simulations to examine the interactions between surfactants and membrane peptides/proteins at different atomic levels. I also collaborate to different multidisciplinary projects with various experimental laboratories in France or abroad to study different systems, such as bacterial photosynthetic centers, peptide-peptide interactions (in amyloid fibrils formation), water dynamics around biomolecules or nanomaterials.

Scientific Production

1. X. Liang, M. Zhang, C. Guo, **S. Abel**, X. Yi, G. Lu, C. Yang and Z. Dang “Competitive solubilization of low-molecular-weight polycyclic aromatic hydrocarbons mixtures in single and binary surfactant micelles” (2014), *Chem. Eng. J.* **244**, 522-530 (IF: 3.47)
2. **S. Abel**, N. Taulier, H. Santuz, W. Urbach and M. Waks. “Aggregation of β -Lactoglobulin Amyloid-Prone Peptides: Effect of Urea and Trehalose: Insights from Molecular Dynamics Simulations”. (2014), *FEBS letter* (accepted) (IF: 3.55)
3. **S. Abel**, A. Lorieau A., B. de Foresta, F-Y Dupradeau and M. Marchi. “Molecular Dynamics Simulations of hMRP1 Transmembrane Peptides in Different Environments”. (2014) *Biochimica et Biophysica Acta*; **1838**(1):493–509 (IF: 4.66)
4. T. Djebaili, J. Richardi, **S. Abel** and M. Marchi. “Atomistic Simulations of the Surface Coverage of Large Gold Nanocrystals”. (2013) *JPCC*; **117**(34):17791–1780. (IF: 4.81)
5. **S. Abel**, F-Y. Dupradeau and M. Marchi. “Molecular Dynamics Simulations of a Characteristic DPC Micelle in Water”. (2012). *JCTC*; **8**(11):4610–4623 (IF: 5.39)
6. **S. Abel**, Dupradeau F-Y, E. P. Raman, A. D. Mackerell Jr. and M. Marchi. “Molecular Simulations of Dodecyl- β -Maltoside Micelle in Water: Headgroup Conformation and the Force Field Parameters”. (2011), *JPCB*; **115**(3):487-99. (IF: 3.61)
7. **S. Abel**, M. Waks and M. Marchi. “Molecular Dynamics Simulations of Cytochrome c unfolding in AOT Reverse Micelles: the first steps”. (2010), *Eur Phys J E Soft Matter*; **32**(4):399-409. (IF: 1.82)
8. **S. Abel**, J. Attia; S. Rémita; M. Marchi; W. Urbach and M. Goldmann. “Atomistic Simulations of Spontaneous Formation and Structural Properties of Linoleic Micelles in water”. (2009), *Chemical Physics Lett.*; **481**(1-3):124-129. (IF:2.15)
9. **S. Abel**, M. Waks; M. Marchi and W. Urbach. “Effect of Surfactant Conformation on the Structures of Small Size Non-Ionic Reverse Micelles, A Molecular Simulation Study”. (2006), *Langmuir*; **22**(22); 9112-20 (IF: 4.19)
11. **S. Abel**, M. Waks; W. Urbach and M. Marchi. “Structure, Stability and Hydration of a Polypeptide in AOT Reverse Micelles”. (2006), *JACS*; **128**(2):382-3. (IF: 10.68)
12. **S. Abel**, F. Sterpone; S. Bandyopadhyay and M. Marchi. “Molecular Modelling and Simulations of AOT-Water Reverse Micelles in Isooctane: Structural and Dynamic Properties”. (2004). *JPCB*; **108**(50):19458–19466. (IF: 3.61)

Books and Chapter

1. **S. Abel** and M. Waks. “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
2. **S. Abel**. *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)

Talks and Posters

More than 15 Talks and Posters in different congress (*e.g.* American Biophysical Meeting, EBSA, CECAM or university and research group workshops).

Reviewing and Evaluation

Regular article reviewer for many academic journals including: *JPCB*, *Langmuir*, *JCTC*, *Molecular Simulation*. Grant evaluations for French universities (2011 - Present).

Teaching and Supervision Responsibilities

I 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.

Areas of Expertise

Expert in fields in molecular biophysics and in computational chemistry with special interests of surfactant and protein systems.

Professional and Scientific Organizations

Member of the American Biophysical Society and the French Biophysical Society (2007-present).