

# Sara Laporte

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## EDUCATION

<b>PhD in computational physics</b>   UNIVERSITY PIERRE AND MARIE CURIE, PARIS	2016
Thesis: "The Electric field at an Oxide Surface – Impact on Reactivity of Prebiotic Molecules"	
Supervisor: A. Marco Saitta	
<b>MSc in condensed matter physics</b>   UNIVERSITY PIERRE AND MARIE CURIE, PARIS	2013
Nanomat specialisation	
Finished top of my year	
<b>BSc</b>   UNIVERSITY OF AUCKLAND, NEW-ZEALAND	2010
Double major Physics and Mathematics	

## RESEARCH EXPERIENCE

<b>CNR-IOM-DEMOCRITOS NATIONAL SIMULATION CENTER C/O SISSA – TRIESTE, ITALY</b>	Sep 2019 – current
Molecular dynamics simulation of the action of anticancer drugs on proteins	
<ul style="list-style-type: none"> <li>• Classical molecular dynamics on large systems ( 500k atoms)</li> <li>• Enhanced sampling and free energy methods</li> </ul>	
<b>INTERNATIONAL SCHOOL OF ADVANCED STUDIES (SISSA) - TRIESTE, ITALY</b>	Dec 2016 – Aug 2019
Simulation of the optical and colour properties of anthocyanins in solution	
<ul style="list-style-type: none"> <li>• Use and refinement of a multiscale protocol developed in the group</li> <li>• Classical and ab-initio molecular dynamics</li> <li>• Enhanced sampling and free energy techniques</li> <li>• Simulation of absorption spectra using time-dependent density functional theory</li> <li>• Development of a method to compute equilibrium constants for prototropic tautomers</li> </ul>	
<b>INSTITUTE OF MINERALOGY, MATERIALS PHYSICS AND COSMOCHEMISTRY - PARIS, FRANCE</b>	Oct 2013 – Oct 2016
Prebiotic reactions at the mineral/water interface - PhD thesis	
<ul style="list-style-type: none"> <li>• Ab-initio molecular dynamics</li> <li>• Metadynamics and umbrella sampling</li> </ul>	

## PUBLICATIONS

"Deciphering the molecular terms of Arp2/3 allosteric regulation from all-atom simulations and dynamical network analysis"	in preparation
S. Laporte, V. Torre and A. Magistrato	
"Molecular mechanisms of the blockage of glioblastoma motility"	under review
J. Xu, F. Simonelli, X. Li, A. Spinello, S. Laporte, V. Torre and A. Magistrato	
Journal of Chemical Information and Modeling	
"The Discovery of a Natural Cyan Blue: A unique food-sourced anthocyanin could replace synthetic Brilliant Blue."	in press
P. R. Denish, J. Fenger, R. Powers, N. Ahmadiani, L. Grisanti, K. G. Guggenheim, S. Laporte, J. Li, T. Kondo, A. Magistrato, M. Moloney, M. Riley, M. Rusishvili, G. T. Sigurdson, S. Baroni, O. Dangles, M. Giusti, T. Collins, J. Didzbalis, K. Yoshida, J. B. Siegel, R. J. Robbins	
Science Advances	

## "Formic Acid Synthesis in a Water-Mineral System: Major Role of the Interface"

S. Laporte, F. Pietrucci, F. Guyot and A.M. Saitta  
The Journal of Physical Chemistry C 129, 5125

2020

## "Unraveling the molecular mechanisms of color expression in anthocyanins"

M. Rusishvili, L. Grisanti, S. Laporte, M. Micciarelli, M. Rosa, R. J. Robbins, T. Collins, A. Magistrato and S. Baroni  
Physical Chemistry Chemical Physics 21, 8757

2019

## "Strong electric fields at a prototypical oxide/water interface probed by ab initio molecular dynamics: MgO(001)"

S. Laporte, F. Finocchi, L. Paulatto, M. Blanchard, E. Balan, F. Guyot and A.M. Saitta  
Physical Chemistry Chemical Physics 17, 20382

2015

## INTERNSHIPS

### INSTITUTE OF MINERALOGY, MATERIALS PHYSICS AND COSMOCHEMISTRY

FEB – JUN 2013

First principles study of water in a carbon nanotube

- Car-Parrinello molecular dynamics using Quantum-Espresso

### INSTITUT DE PHYSIQUE DU GLOBE DE PARIS

JUN – JUL 2013

Statistical signal analysis on geodesic data

- Principal component analysis using MatLab

### UNIVERSITY OF AUCKLAND

JAN – FEB 2010

Evaluation of a phased microphone array

- Field work – data collection
- Statistical signal analysis using MatLab

## TEACHING AND ADMINISTRATIVE DUTIES

### MEMBER OF THE DIRECTIVE BOARD | SISSA CLUB

2020

- Coordination of language courses

### POST-DOC REPRESENTATIVE | SISSA

2018 – 2019

- Elected to represent post-docs of the physics area

### TEACHING ASSISTANT | UNIVERSITY PIERRE AND MARIE CURIE

2013 – 2016

- Tutorials for a first year thermodynamics paper
- Lab demonstrator for a second year spectroscopy paper
- Implementation of exercises on WIMS online teaching platform

### TUTOR | UNIVERSITY OF AUCKLAND

2009 – 2010

- Lab demonstrator
- Tutoring hours in the physics help-room

## SKILLS

### LANGUAGES

Native fluency in French and English  
Italian spoken

### PROGRAMMING

Fortran, C, Matlab, Python

### REFERENCES

Current P.I.:

Alessandra Magistrato [alema \[at\] sissa.it](mailto:alema[at]sissa.it)

Previous P.I.:

Stefano Baroni [baroni \[at\] sissa.it](mailto:baroni[at]sissa.it)

PhD Supervisor:

Marco Saitta [marco.saitta \[at\] sorbonne-universite.fr](mailto:marco.saitta[at]sorbonne-universite.fr)

### INTERESTS

Music:

Brazilian percussion – member of "Banda Berimbau" Trieste  
Member of the SISSA choir

Science Communication:

Ongoing activities with school children within my current institution

Speaker in "Pint of Science" Trieste, May 2017

Participation in short-film festival for PhD students