

# DANIELE LOCO

## PERSONAL INFORMATION

*Born in Italy*, 1 October 1989

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## EDUCATION

*Masters in Chemistry* 2011-2014 Università di Pisa  
Degree Thesis: "Simulation of Excitonic Circular Dichroism spectra in biological molecules".  
Thesis advisor: Prof. Benedetta Mennucci [benedetta.mennucci@unipi.it](mailto:benedetta.mennucci@unipi.it)

*Bachelor in Chemistry* 2008-2011 Università di Pavia  
Degree Thesis: "Correlation Diagrams and Computational Methods in Fotochemistry".  
Thesis advisor: Prof. Angelo Albini [angelo.albini@unipv.it](mailto:angelo.albini@unipv.it)

## COMPUTER SKILLS

*Basic* PYTHON, Microsoft Windows, OpenMP, Haskell

*Intermediate* L<sup>A</sup>T<sub>E</sub>X, OpenOffice, Linux, Shell scripting languages (Bash,Csh)

*Advanced* Fortran

## OTHER INFORMATION

*Grants and awards* 2014-2017 · PhD Fellowship, Università di Pisa

*Latest Conferences and meeting* 2014 · Poster Presentation at the Conference, Pisa. Title: "Simulation of Exciton-Coupled Circular Dichroism spectra of biological molecules"

2015 · Poster Presentation at the Quantum Effects in Biological Systems (QuEBS) Workshops, Firenze. Title: "TD-DFT Exciton Model for Simulating Circular Dichroism Spectra of DNA/RNA and Proteins"

2015 · Poster Presentation at the III National Conference of the Italian Division of Theoretical and Computational Chemistry (DCTC) of the Italian Chemical Society, Roma. Title: "A QM/Excitonic Approach to the Electronic Circular Dichroism of Nucleic Acids"

2017 · Poster Presentation at the Computational Molecular Science 2017 Conference, Warwick. Title: "Born–Oppenheimer Polarizable QM/MM MD: an Extended Lagrangian Formalism"

*Schools* 2015 · European Summer School in Quantum Chemistry, Torre Normanna, Palermo, September 6<sup>th</sup> to September 19<sup>th</sup>

2017 · "Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and Beyond", CECAM, EPFL, Lausanne, Switzerland, May 15<sup>th</sup> to May 19<sup>th</sup>

*Languages* ITALIAN · Mother tongue

ENGLISH · Intermediate (conversationally fluent)

*Interests* Music · Cooking · Chess

*References* Prof. Benedetta Mennucci [benedetta.mennucci@unipi.it](mailto:benedetta.mennucci@unipi.it)

#### PUBLICATIONS

2016 A QM/MM Approach Using the AMOEBA  
Polarizable Embedding: From Ground State Energies to  
Electronic Excitations

*J. Chem. Theory  
Comput.*

Loco, D.; Polack, É.; Caprasecca, S.; Lagardère, L.; Lipparini, F.; Piquemal, J. P.  
and Mennucci, B. ,2016, 12, 3654–3661, DOI: 10.1021/acs.jctc.6b00385

2016 A fast but accurate excitonic simulation of the  
electronic circular dichroism of nucleic acids: how can it be  
achieved?

*Phys. Chem.  
Chem. Phys.*

Loco, D.; Jurinovich, S.; Di Bari, L.; Mennucci, B. ,2016,18, 866-877, DOI:  
10.1039/C5CP06341H

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