Fabio Gabas

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Profile

I am a PhD in theoretical chemistry with a great passion for computer science. My experience in the CINECA supercomputing center has shaped my scientific profile towards deep IT interests.

Currently I am looking for the opportunity to work as Data Scientist or IT consultant in an interesting working environment.

Language Skills

Italian: Native speaker

English: **C1** from **IELTS** certificate

Computer Skills

Program Languages:

C/C++, Fortran, Python, Bash

Operating Systems:

Windows, Linux

Parallel computing:

OpenMP, MPI

Versioning:

GIT

Interests

I like drawing, reading science fiction books, playing cards and playing football with friends

Work Experience

- 2018 - now **PostDoc** at Università degli Studi di Milano
- 2015 - 2018 **PhD** at Università degli Studi di Milano

Development and implementation of new theories for vibrational spectroscopy towards big size systems, within **ERC** Semicomplex project

- 04/2015 - 09/2015: **User Support team** at **SCS**, Technology Transfer of Supercomputing Solutions

Installation of software and tech support for enterprise customers

- 2013 - 2015: **Grant Holder** at **CINECA**

High Performance Computing consulting within Lisa Project
http://www.hpc.cineca.it/services/lisa

Education and Training

- 2010 - 2012: **MS Chemistry**, 110/110 cum Laude at Università degli Studi di Milano

Ab-initio computational thesis: "A quantum mechanics study of halogen bond in C-X/p systems", in partnership with **CNR**

- 2007-2010: **Bachelor in Chemistry**, 110/110 cum Laude at Università degli Studi di Milano

Molecular Dynamics computational thesis: "A Coarse Grained approach for peptide-protein docking: the FtsZ case"

Relevant Publications

- C. Aieta**, F. Gabas**, and M.Ceotto. "Parallel Implementation of Semiclassical Transition State Theory." *Journal of Chemical Theory and Computation* 15.4 (2019): 2142-2153.
- **F. Gabas**, G. Di Liberto, R. Conte, and M. Ceotto. "Protonated Glycine Supramolecular Systems: the need for quantum dynamics" *Chemical Science*, **9** 7894 (2018). "**Pick of the Week**" and **front cover** for an issue of Chemical Science