Alessio Valentini, Ph.D.

I am a passionate researcher who lives at the interface between computer science and computational chemistry. I built my career delivering high quality software to solve chemistry problems. I am an eager learner who enjoys new challenges and tinkers with all things computer science.

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Work Experience:

- **Research Associate/PostDoc at Stanford University.** Project leader and main developer of the Retropaths package, a new software that automates exploration of chemical synthesis channels using graph theory, funded by a multimillion MURI DOD ONR grant *(California 2020-present)*.
- **PostDoc at University of Liège.** Project leader and main developer of a package to perform and analyze quantum dynamics for attosecond time-scale events *(Belgium 2016-2019)*.
- **PostDoc at University of Siena.** Developed tools in the OpenMolcas quantum chemistry suite for semiclassical dynamics and automatic generation of hybrid quantum mechanics / molecular mechanics protein models *(Italy 2015-2016)*.

Skills:

- Developed several Python (**11** years) and Haskell (**3** years) packages for molecular dynamics, reaction discovery, data analysis and data wrangling pipelines.
- Proficiency in developing high performance codes in collaborative settings, as proven by my work in the OpenMolcas suite and in the Martínez group at Stanford University.
- Installed and managed two university clusters for scientific calculations *(2009-2019)*.
- Effective communication skills, with a strong passion for visual effects and 3D rendering, as proven by my 8 presentations and 2 awards at international scientific conferences.

Career achievements:

- Published 22 articles with more than 2400 total citations in peer-reviewed journals in the fields of photochemistry, photobiology, reaction discovery and chemical pedagogy tools.

Education:

- **Ph.D. in Computational Chemistry** on *Semiclassical molecular dynamics*. University of Alcalá, *(Spain 2011-2015)*.
- **M.Sc. in Chemistry** on *Automatic generation of QM/MM models for photoactive proteins*. University of Siena, *(Italy 2008-2011)*.

Python libraries:
Cython
NetworkX
Numpy/Scikit
Pandas
Matplotlib
Rdkit/OpenBabel
Mkdocs

Secondary languages:
CUDA
C/C++
Fortran
React/Javascript

Daily tools:
Bash
VScode
JupyterLab
Docker
CI/CD

Misc:
Blender
Gimp
Inkscape
Latex
d3.js

Real life languages:
Italian
English
Spanish