Alessio Valentini, Ph.D.

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I have been working in computational chemistry for more than 13 years, with a strong emphasis on coding and computer science. I based my career on delivering high quality software to solve chemistry problems, with 22 publications and more than 2400 total citations in the fields of photochemistry, photobiology, reaction discovery and chemical pedagogy tools.
My expertise revolves around molecular dynamics and quantum mechanics calculations, with applications that range from small molecules to proteins, from quantum molecular dynamics propagation to high throughput property screening on molecule databases.

EDUCATION

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

EXPERIENCE

Stanford University Research Associate. *(California 2020-present)*
Keywords: *Reaction discovery. Graph theory. Database screening. Polarizable force fields*.

- Led the *Reactions Template Studio* project as main developer, a software that automates exploration of chemical synthesis channels using graph theory, funded by a multimillion MURI DOD ONR grant. The application can be interfaced with *ab-initio* packages and explore complex networks of chemical reactions, to discover novel synthetic pathways.
- Interfaced scientific C++ and Fortran code bases to implement polarization of QM/MM (quantum mechanics/molecular mechanics) force fields. This implementation enabled GPU acceleration of both QM and MM parts of the calculation to reduce computation time and enable the study of larger systems.
- Developed an Alexa-powered cloud application to perform quantum chemical calculations requested via voice by end users.

Skills: *Python, D3.js, JupyterLab, RdKit, Openeye, NetworkX, CI/CD, AWS, TeraChem, Xtb*.

University of Liège postdoctoral fellow *(Belgium 2016-2019)*
Keywords: *Quantum Dynamics. Attosecond chemistry. Molecular dynamics*.

- Developed Python and Cython implementation of quantum wavepacket propagation. The package solves the time-dependent Schrödinger equation on a 3D grid to allow accurate modelling of highly non-linear light driven processes.
- Delivered C-like performance for complex modelling challenges while providing a user-friendly Python interface. Highly parallel code enabled complex simulations to run quickly and efficiently on modern hardware.
- Analyzed Terabytes of raw data using Python, blender, matplotlib, JupyterLab, numpy, pandas, etc. to produce highly interpretable visualizations of complex quantum phenomena.

Skills: *Python, C++, Cython, Pandas, Numpy, Scikit, CI/CD, OpenMolcas*.

University of Siena postdoctoral fellow *(Italy 2015-2016)*.
Keywords: *Protein design. Mutants discovery. Molecular dynamics*.

- Developed a Python pipeline to automatize generating complex inputs to QM/MM (quantum mechanics / molecular mechanics) simulations.
- Implemented interfaces to multiple computational chemistry packages (ProPKA, Gromacs, Tinker, ...) to allow end users to specify high level scientific objectives, such as PDB screening or protein mutant generation, and get back scientifically-valid insights on emergent properties like florescence or excitation energies.

Skills: *Python, Fortran, Bash, Gromacs, Tinker, OpenMolcas*.

ADDITIONAL SKILLS

- Effective communication, strong passion for visual effects and 3D rendering, as proven by my 8 presentations and 2 awards at international scientific conferences.
- Functional programming enthusiast, with various contributions to Haskell libraries during my PhD, implementing molecular dynamics, data analysis and data wrangling pipelines.
- Strong Linux/Bash/HCP background. Installed and managed two university clusters (50+ nodes) for scientific calculations *(2009-2019)*.
- Firm believer of SOLID principles and clean code practices.

PERSONAL

- Fluent in Italian, English, Spanish.
- Lived in 6 different countries.