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Marc Barbry

Computational Physicist

Summary Ph.D. in Nanoscience with strong experience in the implementation and operation of complex physical models from the molecular up to the device scale (Quantum chemistry, organic electronics, plasmonic) in high performance computing environments.

Profile

- Six years experience in the implementation of scientific software (four focused on Quantum chemistry methods) resulting in six publications in scientific journals
- Implementation of innovative methods in Python, C/C++ and Fortran, e.g., the PyNAO project
- Improvements and parallelization of existing algorithms pushing the limitations of *ab-initio* methods of an order of magnitude
- Implementation of libraries for post data processing and large data manipulations
- Strong written and oral communication skills which led to regional and university scholarships

Professional Experience

May 2020 - present, Metrology Functional Design Engineer; ASML, Veldhoven (the Netherlands)

ASML is the international leader company on photolithography machine bringing the future of electronics devices. My role at ASML consists in participating to the definition of machine level specification of different functions, such as functionality, algorithms, performance and reliability.

May 2018 - April 2020, Technical consultant - Physics; Simbeyond, Eindhoven (the Netherlands)

Simbeyond is a spin-off company focused on the development of organic electronic simulation tools. My responsibilities were

- Technical consulting for customers and prospective customers
- Developing new models for charge transport and photonics in organic electronic devices
- Implementing the models in high performance scientific simulation software
- Providing product training and developing training materials and documentations
- Exploring new application areas for existing simulation software.



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Education

October 2014 - July 2018, PhD in Computational Physics PhD at the Centro de Fisica de Materiales (Spain)

Plasmons in Nanoparticles: Atomistic Ab initio for Large Systems

- Implementation of an efficient algorithm for very large clusters calculations (up to 5000 atoms)
- Study of the induced electric field in nano-cavities
- Electron Energy Loss Spectroscopy (EELS) implementation in a time-dependent density functional theory (TDDFT) code
- Implementation and calculations of Raman spectra

September 2013 - September 2014, M.Sc in Nanoscience Universidad del Pais Vasco (Spain)

First-principles calculation of plasmonic resonances and electric field enhancement in metal-cluster dimers

- Implementation a method to calculate the electric field enhancement of metallic cluster in a TDDFT code, and characterization of the induced field of sodium dimers

September 2012 - August 2013, M.Sc in Photonics Friedrich Schiller Universität (Germany)

Characterization of Guided Second-Harmonic Signal in Lithium Niobate Nanowires by Fourier Imaging

- Construction of optical set-up to characterize the second harmonic generation in lithium niobate nanowires

September 2009 - August 2012, B.Sc in Physics Université de Bordeaux (France)

Implementation of a $O(N^3)$ method of Hedin's GW algorithm for crystal

- Resolution of Quantum mechanics oscillator in Python

Scientific and Software Development Skills

Scientific Skills

- Quantum chemistry methods (DFT, TDDFT, GWA, BSE)
- Algorithm development
- Data analysis
- Plasmonic
- Nanoantennas
- Photonics
- Charge transport in organic electronics
- Excitonics

Programming

- C/C++
- Python
- Fortran
- HTML
- Shell

Software

- Linux
- Git
- Latex
- MPI
- OpenMP
- CUDA

Transferable Skills

- Capacity to work with several projects that resulted in posters and oral contributions in scientific conferences.
- More than six years experience in working in international environments at different companies and research institutes.



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Languages

- French (native)
- English (fluent)
- Spanish (basic)
- German (basic)

Interests

- Quantum chemistry
- Astronomy and astrophotography
- Web development
- Free (as in freedom) software

Publications

- [1] M. Barbry, P. Koval, F. Marchesin, R. Esteban, A. G. Borisov, J. Aizpurua, and D. Sánchez-Portal, “Atomistic Near-Field Nanoplasmonics: Reaching Atomic-Scale Resolution in Nanooptics,” *Nano Letters*, vol. 15, no. 5, pp. 3410–3419, 2015, ISSN: 15306992. DOI: 10.1021/acs.nanolett.5b00759.
- [2] F. Marchesin, P. Koval, M. Barbry, J. Aizpurua, and D. Sánchez-Portal, “Optical response of metallic nanojunctions driven by single atom motion,” *ACS Photonics*, vol. 3, no. 2, pp. 269–277, 2016, ISSN: 2330-4022. DOI: 10.1021/acsp Photonics.5b00609.
- [3] M. Urbieto, M. Barbry, Y. Zhang, P. Koval, D. Sánchez-Portal, N. Zabala, and J. Aizpurua, “Atomic-scale lightning rod effect in plasmonic picocavities: A classical view to a quantum effect,” *ACS Nano*, vol. 12, no. 1, pp. 585–595, 2018. DOI: 10.1021/acsnano.7b07401.
- [4] P. Koval, M. Barbry, and D. Sánchez-Portal, “Pyscf-nao: An efficient and flexible implementation of linear response time-dependent density functional theory with numerical atomic orbitals,” *Computer Physics Communications*, vol. 236, pp. 188–204, 2019, ISSN: 0010-4655. DOI: <https://doi.org/10.1016/j.cpc.2018.08.004>.
- [5] S. Gottardi, M. Barbry, R. Coehoorn, and H. van Eersel, “Efficiency loss processes in hyperfluorescent oleds: A kinetic monte carlo study,” *Applied Physics Letters*, vol. 114, no. 7, p. 073301, 2019. DOI: 10.1063/1.5079642.
- [6] Q. Sun, X. Zhang, S. Banerjee, P. Bao, M. Barbry, N. S. Blunt, N. A. Bogdanov, G. H. Booth, J. Chen, Z.-H. Cui, J. J. Eriksen, Y. Gao, S. Guo, J. Hermann, M. R. Hermes, K. Koh, P. Koval, S. Lehtola, Z. Li, J. Liu, N. Mardirossian, J. D. McClain, M. Motta, B. Mussard, H. Q. Pham, A. Pulkin, W. Purwanto, P. J. Robinson, E. Ronca, E. R. Sayfutyarova, M. Scheurer, H. F. Schurkus, J. E. T. Smith, C. Sun, S.-N. Sun, S. Upadhyay, L. K. Wagner, X. Wang, A. White, J. D. Whitfield, M. J. Williamson, S. Wouters, J. Yang, J. M. Yu, T. Zhu, T. C. Berkelbach, S. Sharma, A. Y. Sokolov, and G. K.-L. Chan, “Recent developments in the pyscf program package,” *The Journal of Chemical Physics*, vol. 153, no. 2, p. 024109, 2020. DOI: 10.1063/5.0006074.
- [7] M. Barbry, P. Koval, and D. Sánchez-Portal, “Ab initio atomistic theory of electron energy loss spectroscopy,” (*Submitted*), 2020.