

Alexandr Fonari

School of Chemistry & Biochemistry and Center for Organic Photonics and Electronics

Georgia Institute of Technology, Atlanta, GA, USA

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QUALIFICATIONS and INTERESTS

- Trained theoretical and computational physicist
- 10 years experience Fortran, C, Python, PERL, PHP
- Skilled in parallel computing (MPI, OpenMP)
- Interested in computational materials and pharma/biotech
- Involved in the development of scientific software
- Permanent resident of United States

EDUCATION

Georgia Institute of Technology

Ph.D. – Computational Physical Chemistry – GPA: 3.77/4.00

Atlanta, GA, USA

2011 – July 2015

- Co-authored 10 peer-reviewed publications
- Recipient of 2015 COPE Graduate Fellowship: 4 winners from total of 250 students are awarded
- Presented 2 contributed talks at international conferences

New Mexico Highlands University

M.Sc. – Applied Chemistry – GPA: 3.88/4.00

Las Vegas, NM, USA

2009 – 2011

- Co-authored 12 peer-reviewed publications
- Phi Kappa Phi

Moldova State University

B.Sc. – Theoretical Physics – GPA: 8.40/10.00

Chisinau, Moldova

2006 – 2009

- Instructed Computer Science I (2008)

EXPERIENCE

Georgia Institute of Technology

Graduate Research Assistant

Atlanta, GA, USA

2011 – Present

- Successfully modeled electrical conductivity and charge-carrier mobility in organic semiconductors within multidisciplinary collaboration of 5 research groups, resulting in 2 *Nature Communications* publications.
- Implemented computational screening of organic semiconductors using a combination of DFT and molecular dynamics, resulting in a *Journal of the American Chemical Society* publication, cited by 20 researchers.
- Administered technical support for a research group of 15 people in compiling and exploring a wide range of electronic-structure packages (VASP, Quantum-Espresso, CRYSTAL, NWChem, Q-Chem, Gaussian, etc.) on Linux-based high-performance supercomputers: Cray and SGI.

New Mexico Highlands University

Graduate Research Assistant/Research Technician at the X-Ray Facility

Las Vegas, NM, USA

2009 – 2011

- Provided structural characterization and identified binding sites in several metal-organic frameworks, resulting in higher storage concentrations of the hydrogen gas (H₂) in one of the derived systems.
- Administered training and technical support in using Bruker SMART APEX II single-crystal diffractometer to staff and students (20+ people) of the Department of Biology and Chemistry.

Gorasoftware S.R.L.

Junior Web Developer

Chisinau, Moldova

2005 – 2006

- Developed a complete virtual messaging system with possibilities of sending, receiving and drafting messages between users using PHP with Smarty template engine and MySQL database.
- Successfully integrated messaging system into the parent social network, resulting in an improved experience for users.

SOFTWARE PROJECTS

Raman Spectra Database of Inorganic Materials

Implemented in Python using VASP as a back-end and Django database interface

Georgia Tech

2014 – Present

- Developed Raman spectrum simulator for crystals and thin-films: github.com/raman-sc.
- Implemented automated workflow to: calculate Raman spectrum of an inorganic material employing job scheduling system (PBS/TORQUE), populate database using Python/Django db module, compare with experimental spectra (when available).
- This implementation is used by at least 5 outside research groups.

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SOFTWARE PROJECTS CONTD.

First-principles evaluation of the electron coupling in condensed phase morphology

Georgia Tech

Implemented in Fortran and Python

2013 – 2014

- Developed a highly parallel implementation of the electronic coupling evaluation employing GlobalArrays in the NWChem program (5M lines): www.nwchem-sw.org.
- Implemented automated workflow to: extract geometries from molecular dynamics snapshots, calculate electronic couplings, compute distributions (Python/numpy/scipy), and visualize the results (Python/matplotlib).
- Results obtained using this implementation are published in several peer-reviewed publications: [10.1002/chem.201303308](https://doi.org/10.1002/chem.201303308), [10.1021/cm503439r](https://doi.org/10.1021/cm503439r).

Interface between Quantum-ESPRESSO program (Fortran) and libpspio library (C)

Georgia Tech

Implemented in Fortran and C

2013 – 2014

- Successfully interfaced libpspio (3K lines) with Quantum-ESPRESSO (500K lines), resulting in the ability of Quantum-ESPRESSO to read/write different pseudopotential file formats.
- Interfacing consisted in: modification of autoconf/Makefile, developing of a suitable C interface, and modification of the Fortran code to call C functions ([Github](#)).
- This implementation allows better interoperability between Quantum-ESPRESSO and other electronic-structure codes, resulting in improved portability and reproducibility.

Effective Mass Calculator for Periodic Systems

Georgia Tech

Implemented in Python and Fortran using VASP or CRYSTAL as back-ends

2011 – 2014

- Developed a highly portable implementation of the effective mass evaluation in crystals: [Github](#).
- Algorithm consists in: defining finite-difference grid, evaluating 2nd order energy derivatives on three or five-point stencil, and diagonalizing the energy tensor.
- At least 3 outside research groups are using this implementation, it was cited 10 times.

VOLUNTEERING

- Presented working principles of organic solar cells for middle school students (40+ students) at *GT Future Tech 2014* and *GT Future Tech 2015* events (Atlanta, GA, USA).
- Invited judge of the undergraduate poster competition at the Southeast Regional Meeting of the American Chemical Society. Assessed research and presentation of 120 posters (Nov. 12-16, 2013, Atlanta, GA, USA).
- Demonstrated working principles of organic electronic devices for middle school students (50+ students) at the West Las Vegas Middle School (2011, Las Vegas, NM, USA): [webpage](#).
- Organized Linux festival (100+ people) for Linux.MD project. Managed technical and administrative teams (2008, Chisinau, Moldova).

MOST SIGNIFICANT PUBLICATIONS

- A. A. Bakulin, R. Lovrincic, Y. Xi, O. Selig, H. J. Bakker, Y. L.A. Rezus, P. K. Nayak, **A. Fonari**, *et al.*, "Mode-selective vibrational modulation of charge transport in organic electronic devices", *Nature Communications* (2015): *accepted* ([arXiv/1503.00777](https://arxiv.org/abs/1503.00777))
- K. Goetz, **A. Fonari**, *et al.*, "Freezing-in Orientational Disorder Induces Crossover from Thermally Activated to Temperature-Independent Transport in Organic Semiconductors", *Nature Communications* (2014): [10.1038/ncomms6642](https://doi.org/10.1038/ncomms6642)
- A. Fonari** *et al.*, "Impact of Exact Exchange in the Description of the Electronic Structure of Organic Charge-Transfer Molecular Crystals", *Physical Review B* (2014): [10.1103/PhysRevB.90.165205](https://doi.org/10.1103/PhysRevB.90.165205)
- L. Zhang, **A. Fonari**, *et al.*, "Bistetracene: An Air-Stable, High-Mobility Organic Semiconductor with Extended Conjugation", *Journal of the American Chemical Society* (2014): [10.1021/ja503643s](https://doi.org/10.1021/ja503643s). [Front cover](#)
- A. Fonari** *et al.*, "On Justification of Cu(II) Environment in Mononuclear Complexes: Joint X-ray and AIM Studies", *Polyhedron* (2011): [10.1016/j.poly.2011.04.002](https://doi.org/10.1016/j.poly.2011.04.002)
- ★ **Total: 21 peer-reviewed publications, cited 122 times, h-index is 6:** [Google Scholar profile](#)