

# Alexandr Fonari

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

Georgia Institute of Technology, Atlanta, GA, USA

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## SUMMARY

Demonstrated experience in modeling physical processes using numerical methods. Applied regression methods to analyze unordered data. Implemented required mathematical formalisms in large code bases and from scratch, using both static and dynamic-typed languages. Successfully collaborated within multidisciplinary and multinational research teams.

- 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 Chemistry – GPA: 3.77/4.00

Atlanta, GA, USA

July 2015

### New Mexico Highlands University

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

Las Vegas, NM, USA

2011

### Moldova State University

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

Chisinau, Moldova

2009

## EXPERIENCE

### Georgia Institute of Technology

Graduate Research Assistant

Atlanta, GA, USA

2011 – Present

Conducted high-quality research in the area of organic electronics. 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.

#### Accomplishments:

- 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.
- Co-authored 10 peer-reviewed publications. Presented 2 contributed talks at international conferences.

### New Mexico Highlands University

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

Las Vegas, NM, USA

2009 – 2011

Collected diffraction data, solved and refined over 100 crystal structures of organic crystals and metal-organic frameworks. 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.

#### Accomplishments:

- Provided structural characterization and identified binding sites in several metal-organic frameworks, resulting in higher storage concentrations of the hydrogen gas (H<sub>2</sub>) in one of the derived systems.
- Analyzed Cambridge Crystallographic Database for bonding topologies in copper mononuclear complexes, resulting in a *Polyhedron* publication
- Co-authored 12 peer-reviewed publications.

### Gorasoftware S.R.L.

Junior Web Developer

Chisinau, Moldova

2005 – 2006

Developed and tested front-end (HTML/JavaScript) and back-end (PHP/MySQL) of web applications. Created requirements and specifications. Communicated accurately with Billing and Finance. Worked closely with UI and UX designers. Presented to senior management progress and goals.

#### Accomplishments:

- 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 user experience.

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## SOFTWARE PROJECTS

### Raman Spectra Database of Inorganic Materials

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

- Developed a highly portable Raman spectrum simulator for crystals and thin-films: [github.com/raman-sc](https://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.

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

*Implemented in Fortran and Python*

- Developed a highly parallel implementation of the electronic coupling evaluation employing GlobalArrays in the NWChem program (5M lines): [www.nwchem-sw.org](http://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 libspio library (C)

*Implemented in Fortran and C*

- Successfully interfaced libspio (3K lines) with Quantum-ESPRESSO (500K lines), resulting in its ability 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](https://github.com)).
- This implementation allows better interoperability between Quantum-ESPRESSO and other electronic-structure codes, resulting in improved portability and reproducibility.

## VOLUNTEERING and COMMUNITY WORK

### FutureTech | Georgia Tech

*Demonstrator*

Atlanta, GA, USA

2014 – 2015

Demonstrated working principles of organic solar cells for middle school students (40+ students). Prepared and tested demonstration and exhibition equipment for conference presentations.

### Linux.MD project

*Event Coordinator*

Chisinau, Moldova

2007 – 2009

Co-Organized outdoor Linux conference (100+ people). Managed technical and administrative teams. Set-up wireless network. Ensured availability of equipment and electricity. Led the organization of Ubuntu InstallFest (50+ people).

## 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](#)