

# 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 Center for Organic Photonics and Electronics Graduate Student Fellowship

### 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*

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 (H<sub>2</sub>) 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](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.

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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 in the NWChem program (5M lines).
- Implemented automated workflow to: extract geometries from molecular dynamics snapshots, calculate electronic couplings, compute statistics (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 of: modification of autoconf/Makefile, developing of a suitable C interface, 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.

## 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](#))
- 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](#)

## ORAL PRESENTATIONS

- A. Fonari** *et al.*, "Joint Mean-Field and Ab Initio Study of the Exciton Dynamics Due to Low-Energy Phonons in Rubrene Single Crystal", Materials Research Society (MRS) Fall Meeting, Nov. 30-Dec. 5, 2014, Boston, MA, USA
- A. Fonari** *et al.*, "The Impact of Exact Exchange Energy in Describing the Charge-Transport Properties in Organic Charge-Transfer Semiconductors", International Conference on the Physics of Semiconductors (ICPS), Aug. 10-15, 2014, Austin, TX, USA

## THESES

- Ph.D.** Thesis: "Theoretical Description of Charge Transport and Exciton Fission in Single-Component and Bimolecular Charge-Transfer Organic Semiconductors", advisors: Veaceslav Coropceanu and Jean-Luc Bredas, *in preparation*
- M.Sc.** Thesis: "X-Ray Diffraction and Computational Studies of Materials for Photonics and Electronic Applications", advisors: Mikhail Yu. Antipin and Tatiana V. Timofeeva
- B.Sc.** Thesis: "Theoretical Investigations of Crossover Effects in Fe(II) Ions", advisor: Sophia I. Klokishner