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 — **Atlanta, GA, USA**
Ph.D. – Computational Physical Chemistry – GPA: 3.77/4.00 — *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 — **Las Vegas, NM, USA**
M.Sc. – Applied Chemistry – GPA: 3.88/4.00 — *2009 – 2011*

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

Moldova State University — **Chisinau, Moldova**
B.Sc. – Theoretical Physics – GPA: 8.40/10.00 — *2006 – 2009*

- Instructed Computer Science I (2008)

EXPERIENCE

Georgia Institute of Technology — **Atlanta, GA, USA**
Graduate Research Assistant — *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 — **Las Vegas, NM, USA**
Graduate Research Assistant — *2009 – 2011*

- Provided structural characterization and identified binding sites in several metal-organic frameworks, resulting in higher storage concentrations of the hydrogen gas (H_2) 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.

Gorasoft S.R.L. — **Chisinau, Moldova**
Junior Web Developer — *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 — **Georgia Tech**
Implemented in `Python` *using* `VASP` *as a back-end and* `Django` *database interface* — *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 in the `NWChem` program (5M lines): www.nwchem-sw.org.
- 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, 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
- **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
- 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. 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

⋆ **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