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 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*

- 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**
M.Sc. – Applied Chemistry – GPA: 3.88/4.00 *2009 – 2011*

- Provided structural characterization of materials for hydrogen storage and catalysis via single-crystal diffraction as a part of collaboration with *Los Alamos National Laboratory*
- Administered training and technical support to staff and students (20+ people) of the Department of Biology and Chemistry in using Bruker SMART APEX II single-crystal diffractometer

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

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 high-throughput calculation of Raman spectra of inorganic materials by combining Python/Django `db` module with job scheduling system (`PBS/TORQUE`) on cluster/supercomputer
- The implementation runs in background, is highly portable and has simple stop/restart functionality, important for busy supercomputer environment

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` package
- Implemented automated workflow to: extract geometries from molecular dynamics snapshots, calculate electronic couplings from pairs and compute statistics using `Python/numpy/scipy`
- Results obtained using this implementation are published in several peer-reviewed publications: 10.1002/chem.201303308, 10.1021/cm503439r

Messaging system within a web-portal/social network **Gorasoft S.R.L.**
Implemented in `PHP/MySQL` *with* `Smarty` *template system* *2005 – 2006*

- Developed a complete virtual messaging system, with possibilities of receiving, composing and drafting messages between users
- Messaging system was deeply integrated and was playing a key role within the parent social network

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PROFESSIONAL DEVELOPMENT TRAINING

- *Extended Software Development Workshop* at CECAM-EPFL (Summer 2014, Lausanne, Switzerland)
  - Interfaced the `libpspio` library (`C`) with the `Quantum-ESPRESSO` package (`Fortran`): modified `autoconf/Makefile`, developed suitable (`C`) interface, modified Fortran code to call `C` functions (Github)
- *Advanced Quantum-ESPRESSO Developer Training* at SISSA (Winter 2013, Trieste, Italy)
  - Converted legacy module of `Quantum-ESPRESSO` package (`Fortran`) to the current version: team of 12 people, 10 days, 10k lines of code

LEADERSHIP and AWARDS

- Recipient of *2015 Center for Organic Photonics and Electronics Graduate Student Fellowship*
- Supervised the research of undergraduate students which resulted in several peer-reviewed publications: 10.1021/jp502411u, 10.1021/cg500284q, 10.1016/j.molstruc.2011.09.032
- Instructed Computer Science I (2008), Quantitative Analysis (2010), General Chemistry I (2011)
- Volunteered at *GT Future Tech 2014* event for middle school students (Spring 2014, Atlanta, GA, USA)

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
- S. K. Mohapatra, **A. Fonari**, *et al.*, "Dimers of Nineteen-Electron Sandwich Compounds: Crystal and Electronic Structures, and Comparison of Reducing Strengths", Chemistry – A European Journal (2014): 10.1002/chem.201404007. Back cover
- 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:** 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