Alexandr Fonari

School of Chemistry & Biochemistry and Center for Organic Photonics and Electronics
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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 **Atlanta, GA, USA**
Ph.D. – Computational Chemistry – GPA: 3.77/4.00 *July 2015*
- Recipient of *2015 COPE Graduate Fellowship*: 4 winners are awarded from total of 250 students

New Mexico Highlands University **Las Vegas, NM, USA**
M.Sc. – Applied Chemistry – GPA: 3.88/4.00 *2011*

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

EXPERIENCE

Georgia Institute of Technology **Atlanta, GA, USA**
Graduate Research Assistant *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 **Las Vegas, NM, USA**
Graduate Research Assistant/Research Technician at the X-Ray Facility *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_2) in one of the derived systems.
- Analyzed Crystallographic Database for bonding topologies, resulting in a *Polyhedron* publication
- Co-authored 12 peer-reviewed publications.

Gorasoft S.R.L. **Chisinau, Moldova**
Junior Web Developer *2005 – 2006*

Developed and tested front-end (`HTML/Java Script`) 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.
- 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.
- 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, 10.1021/cm503439r.

Interface between `Quantum-ESPRESSO` program (`Fortran`) and `libpspio` library (`C`)
Implemented in `Fortran` *and* `C`

- Successfully interfaced `libpspio` (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).
- 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 — **Atlanta, GA, USA**
Demonstrator — *2014 – 2015*
Prepared and tested demonstration and exhibition equipment for conference presentations. Demonstrated working principles of organic solar cells for middle school students (40+ students).

Linux.MD project — **Chisinau, Moldova**
Event Coordinator — *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)
- 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