


# Alexandr Fonari

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

Georgia Institute of Technology, Atlanta, GA, 30332-0400, USA

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## SUMMARY OF QUALIFICATIONS

- Trained theoretical and computational physicist
- Scientific software developer (Fortran, C, Python, PERL)
- Experienced single-crystal X-ray crystallographer
- Skilled in HPC technologies (MPI, OpenMP, GlobalArrays)
- Interested in electronic structure of materials
- Permanent resident of United States (*anticipated July 2015*)

## EDUCATION

### Georgia Institute of Technology

Atlanta, GA, USA

Ph.D. – Theoretical Physical Chemistry – GPA: 3.77/4.00

2011 – July 2015

- Modeled charge transport in molecular semiconductors using a combination of DFT and molecular dynamics simulations
- Interfaced Python and VASP to compute Raman spectra in single crystals: [github.com/raman-sc](https://github.com/raman-sc)
- Identified advantageous structure-property relationships of prospective organic materials for applications in electronics and photonics
- Compiled and explored electronic-structure packages (VASP, Quantum-Espresso, CRYSTAL, NWChem, Q-Chem, Gaussian etc.) on high-performance supercomputers (HPCs) such as Cray and SGI

### New Mexico Highlands University

Las Vegas, NM, USA

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

2009 – 2011

- Collected diffraction data, solved and refined over 100 crystal structures of organic crystals and metal-organic frameworks
- Surveyed and statistically analyzed Cambridge Crystallographic Database for bonding topologies in organic crystals
- Administered and supported Bruker® SMART APEX II CCD single-crystal diffractometer

### Moldova State University

Chisinau, Moldova

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

2006 – 2009

## PROJECTS

### Electronic Structure Library (ESL) initiative

Community-maintained repository of software for use in electronic structure simulations

2014 – Present

- The aspiration of the ESL initiative is to combine open-source libraries that can be used as the building blocks for assembling full-fledged electronic structure packages
- Within ESL, I have interfaced the libbspio library with the Quantum-ESPRESSO package
- Quantum-ESPRESSO interfaced with libbspio is able to read/write different pseudopotential formats
- ★ ESL initiative website: [esl.cecam.org](http://esl.cecam.org)

### High-throughput electronic coupling calculations in organic semiconductors

Open-source implementation in Fortran integrated in the NWChem package

2013 – 2014

- Electronic coupling is a key microscopic parameter in the description of the charge-transport properties of organic semiconductors
- I have programmed a highly parallelized implementation of the electronic coupling evaluation in the NWChem package
- This implementation allows calculation of the electronic couplings in large systems (> 1000 atoms), it is only limited by RAM memory available on the machine
- ★ Project website: [nwchem-sw.org](http://nwchem-sw.org)

### Engineering of new organic semiconductors based on nonlinear fused acenes

Joint effort of multi-disciplinary team from Georgia Tech, Univ. of Massachusetts, and Univ. of Kentucky

2013 – 2014

- Acenes are prototypical organic semiconductors consisting of fused benzene rings
- I have modeled the electronic structure and stabilities of several promising extended nonlinear acenes
- Based on my studies, several novel acenes with significant hole mobilities have been engineered

## PROFESSIONAL DEVELOPMENT TRAINING

- Extended Software Development Workshop at CECAM-EPFL (Summer 2014, Lausanne, Switzerland)
- Advanced Quantum-ESPRESSO Developer Training at SISSA (Winter 2013, Trieste, Italy)
- Hooked on Photonics sponsored by National Science Foundation at Georgia Tech (Summer 2010, Atlanta, GA, USA)

## MENTORING and LEADERSHIP

- Supervised the research of undergraduate students which resulted in the following peer-reviewed publications:
  1. Nathan S. Corbin – J. Phys. Chem. C (2014): [10.1021/jp502411u](https://doi.org/10.1021/jp502411u)
  2. Bhupinder Sandhu – Cryst. Growth Des. (2014): [10.1021/cg500284q](https://doi.org/10.1021/cg500284q)
  3. Joel Zazueta – J. Mol. Struct. (2011): [10.1016/j.molstruc.2011.09.032](https://doi.org/10.1016/j.molstruc.2011.09.032)
- Teaching assistant: Computer Science I (2008), Quantitative Analysis (2010), General Chemistry I (2011)

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## PEER-REVIEWED PUBLICATIONS ([Google Scholar profile](#))

1. L. Stevens, K. Goetz, **A. Fonari**, *et al.*, "Temperature Mediated Polymorphism in Molecular Crystals: The Impact on Crystal Packing and Charge Transport", *Chem. Mater.* (2014): [10.1021/cm503439r](#)
2. K. Goetz, **A. Fonari**, *et al.*, "Freezing-in orientational disorder induces crossover from thermally activated to temperature-independent transport in organic semiconductors", *Nat. Commun.* (2014): [10.1038/ncomms6642](#)
3. **A. Fonari** *et al.*, "Impact of Exact Exchange in the Description of the Electronic Structure of Organic Charge-Transfer Molecular Crystals", *Phys. Rev. B* (2014): [10.1103/PhysRevB.90.165205](#)
4. S. K. Mohapatra, **A. Fonari**, *et al.*, "Dimers of Nineteen-Electron Sandwich Compounds: Crystal and Electronic Structures, and Comparison of Reducing Strengths", *Chem. Eur. J.* (2014): [10.1002/chem.201404007](#). [Back cover](#)
5. **A. Fonari** *et al.*, "Toward Antikekulene: Angular 1,2-Di-, 2,3-Di-, and 1,2,15,16-Tetrachloro[6]phenylene", *Synlett* (2014): [10.1055/s-0034-1379140](#)
6. L. Zhu, Y. Yi, **A. Fonari**, *et al.*, "Electronic Properties of Mixed-Stack Organic Charge-Transfer Crystals", *J. Phys. Chem. C* (2014): [10.1021/jp502411u](#)
7. V. N. Khrustalev, B. Sandhu, S. Bentum, **A. Fonari**, *et al.*, "Absolute Configuration and Polymorphism of 2-Phenylbutyramide and  $\alpha$ -Methyl- $\alpha$ -phenylsuccinimide", *Cryst. Growth Des.* (2014): [10.1021/cg500284q](#)
8. L. Zhang, **A. Fonari**, *et al.*, "Bistetracene: An Air-Stable, High-Mobility Organic Semiconductor with Extended Conjugation", *J. Am. Chem. Soc.* (2014): [10.1021/ja503643s](#). [Front cover](#)
9. L. Zhang, **A. Fonari**, *et al.*, "Triisopropylsilylethynyl-Functionalized Graphene-Like Fragment Semiconductors: Synthesis, Crystal Packing, and Density Functional Theory Calculations", *Chem. Eur. J.* (2013): [10.1002/chem.201303308](#). [Back cover](#)
10. A. R. Morales, A. Frazer, A. W. Woodward, H.-Y. Ahn-White, **A. Fonari**, *et al.*, "Design, Synthesis, and Structural and Spectroscopic Studies of Push-Pull Two-Photon Absorbing Chromophores with Acceptor Groups of Varying Strength", *J. Org. Chem.* (2013): [10.1021/jo302423p](#)
11. E. S. Leonova, N. S. Makarov, **A. Fonari**, *et al.*, "Synthesis, structure, and one- and two-photon absorption properties of N-substituted 3,5-bisarylidenepropenepiperidin-4-ones", *J. Mol. Struct.* (2013): [10.1016/j.molstruc.2012.12.034](#)
12. A. O. El-Ballouli, R. S. Khnayzer, J. C. Khalife, **A. Fonari**, *et al.*, "Diarylpyrenes vs. Diaryltetrahydropyrenes: Crystal Structures, Fluorescence, and Upconversion Photochemistry", *J. Photochem. Photobiol. A* (2013): [10.1016/j.jphotochem.2013.07.018](#)
13. B. R. Kaafarani, A. O. El-Ballouli, R. Trattnig, **A. Fonari**, *et al.*, "Bis(carbazolyl) Derivatives of Pyrene and Tetrahydropyrene: Synthesis, Structures, Optical Properties, Electrochemistry, and Electroluminescence", *J. Mater. Chem. C* (2013): [10.1039/c2tc00474g](#). [Most Accessed Manuscripts for J. Mater. Chem. C in 2013](#)
14. I. V. Magedov, N. M. Evdokimov, A. S. Peretti, M. Karki, D. T. Lima, L. Frolova, M. R. Reisenauer, A. E. Romero, P. Tongwa, **A. Fonari**, *et al.*, "Reengineered Epipodophyllotoxin", *Chem. Commun.* (2012): [10.1039/c2cc35044k](#)
15. L. E. Polander, L. Pandey, A. Romanov, **A. Fonari**, *et al.*, "2,6-Diacynaphthalene-1,8:4,5-Bis(dicarboximides): Synthesis, Reduction Potentials, and Core Extension", *J. Org. Chem.* (2012): [10.1021/jo300623z](#)
16. I. V. Kosilkin, E. A. Hillenbrand, P. Tongwa, **A. Fonari**, *et al.*, "Synthesis, Structure, Thermal and Nonlinear Optical Properties of a Series of Novel D- $\pi$ -A Chromophores with Varying Alkoxy Substituents", *J. Mol. Struct.* (2011): [10.1016/j.molstruc.2011.09.032](#)
17. **A. Fonari** *et al.*, "Experimental and Theoretical Structural Study of (3E,5E)-3,5-bis-(benzylidene)-4-oxopiperidinium Mono- and (3E,5E)-3,5-bis-(4-N,N-dialkylammonio)benzylidene)-4-oxopiperidinium Trications", *J. Mol. Struct.* (2011): [10.1016/j.molstruc.2011.06.020](#)
18. **A. Fonari** *et al.*, "Two Polymorphs of Phenanthro[4,5-*abc*]phenazine-18-crown-6: Preparation, X-ray Diffraction and DFT Studies", *J. Mol. Struct.* (2011): [10.1016/j.molstruc.2011.04.039](#)
19. **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](#)
20. E. S. Leonova, M. V. Makarov, E. Y. Rybalkina, S. L. Nayani, P. Tongwa, **A. Fonari**, *et al.*, "Structure-Cytotoxicity Relationship in a Series of N-phosphorus Substituted *E,E*-3,5-bis(3-pyridinylmethylene)- and *E,E*-3,5-bis(4-pyridinylmethylene)piperid-4-ones", *Eur. J. Med. Chem* (2010): [10.1016/j.ejmech.2010.09.058](#)

## SELECTED ORAL PRESENTATIONS

1. **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
2. **A. Fonari** *et al.*, *The Impact of Exact Exchange Energy in Describing the Charge-Transport Properties in Organic Charge-Transfer Semiconductors*, 32<sup>nd</sup> International Conference on the Physics of Semiconductors (ICPS), Aug. 10-15, 2014, Austin, TX, USA

## THESES

- **Ph.D.** Thesis: *Theoretical Characterization of Charge Transport of Extended Acenes and 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.