Alexandr Fonari

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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
- 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 `libpspio` library with the `Quantum-ESPRESSO` package
- `Quantum-ESPRESSO` interfaced with `libpspio` is able to read/write different pseudopotential formats
- ⋆ ESL initiative website: 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

Engineering of new organic semiconductors based on extended annulated oligoacenes

Joint effort of multi-disciplinary team from Georgia Tech, Univ. of Massachusetts, and Univ. of Kentucky — *2013 – 2014*

- Oligoacenes are prototypical organic semiconductors consisting of fused benzene rings
- I have modeled the electronic structure and stabilities of several promising extended oligoacenes
- Based on my studies, several novel oligoacenes with high 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
  2. Bhupinder Sandhu – Cryst. Growth Des. (2014): 10.1021/cg500284q
  3. Joel Zazueta – J. Mol. Struct. (2011): 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. **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): *accepted*
2. 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
3. **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
4. 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
5. V. N. Khrustalev, B. Sandhu, S. Bentum, **A. Fonari**, *et al.*, "Absolute Configuration and Polymorphism of 2-Phenylbutyramide and α-Methyl-α-phenylsuccinimide", Cryst. Growth Des. (2014): 10.1021/cg500284q
6. 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
7. 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
8. 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
9. E. S. Leonova, N. S. Makarov, **A. Fonari**, *et al.*, "Synthesis, structure, and one- and two-photon absorption properties of N-substituted 3,5-bisarylidene*propen*piperidin-4-ones", J. Mol. Struct. (2013): 10.1016/j.molstruc.2012.12.034
10. 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
11. 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
12. 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
13. L. E. Polander, L. Pandey, A. Romanov, **A. Fonari**, *et al.*, "2,6-Diacylnaphthalene-1,8:4,5-Bis(dicarboximides): Synthesis, Reduction Potentials, and Core Extension", J. Org. Chem. (2012): 10.1021/jo3006232
14. 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-π-A Chromophores with Varying Alkoxy Substituents", J. Mol. Struct. (2011): 10.1016/j.molstruc.2011.09.032
15. **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
16. **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
17. **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
18. 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 and POSTER PRESENTATIONS

1. Oral: **A. Fonari**, *et al.*, *The Impact of Exact Exchange Energy in Describing the Charge-Transport Properties in Organic Charge-Transfer Semiconductors*, 32^{nd} International Conference on the Physics of Semiconductors (Aug. 10-15, 2014, Austin, TX, USA)
2. Oral: **A. Fonari**, *et al.*, *The Influence of the Hartree-Fock Exchange on the Charge-Transport Characteristics in Organic Crystalline Semiconductors*, Southeast Theoretical Chemistry Association Meeting (May 15-17, 2014, Atlanta, GA, USA)

THESES

- **Ph.D.** Thesis: *Theoretical Characterization of the Charge Transport of Extended Oligoacenes 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.