

# Alona Furmanchuk, PhD

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## ACADEMIC APPOINTMENTS

- 2016-Now Research Associate, Center for Health Information Partnership, Northwestern University, Chicago, IL
- 2015-2016 Research Associate, Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, IL
- 2012-2015 Research Associate, Department of Chemistry, Northwestern University, Evanston, IL
- 2010-2011 Postdoctoral Fellow, Interdisciplinary Center for Nanotoxicity, Jackson State University, Jackson, MS

## HONORS AND AWARDS

- 2015 ACS Physical Chemistry Division Postdoctoral Research Award
- 2010 Exemplary Doctoral Scholar
- 2009 2nd best poster presentation award. 18th Conference on Current Trends in Computational Chemistry, Jackson MS
- 2008 3rd best poster presentation award. 17th Conference on Current Trends in Computational Chemistry, Jackson MS
- 2005 2nd best poster presentation award. 14th Conference on Current Trends in Computational Chemistry, Jackson MS

## EDUCATION

- |      |      |  |           |
|------|------|--|-----------|
| Ph.D | 2010 | Jackson State University, Jackson, MS, USA               | Chemistry |
| M.S  | 2002 | Dnipropetrovsk State University, Dnepropetrovsk, Ukraine | Chemistry |

## TRAINING

- 2010 Computational Biophysics Workshops, Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign, San Diego CA,
- 2009 Summer Internship, Theoretical Division, Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM,
- 2006 Bioinformatics and Sequence Analysis Workshop, Tennessee State University, Nashville TN

## COMMUNITY/PUBLIC SERVICE

Habitat for Humanity

## PARTICIPATION IN PROFESSIONAL SOCIETIES AND EXTRAMURAL ORGANIZATIONS

Member of American Chemical Society

## EDITORIAL AND MANUSCRIPT REVIEW RESPONSIBILITIES

The Journal of Physical Chemistry  
Journal of Molecular Modeling  
Structural Chemistry (STUC)  
CARBON  
Soft Matter

## PUBLICATIONS AND SCHOLARY WORK

### A. Peer-reviewed Original Investigations

1. Machine learning for improving performance of organic photovoltaics. Arindam Paul, Al'ona Furmanchuk, Wei-keng Liao, Alok Choudhary, Ankit Agrawal. *In progress*.
2. Prediction of Seebeck coefficient for non-stoichiometric compounds: A machine learning approach. Furmanchuk, Al'ona, Agrawal, Ankit, Saal, James, Doak, Jeff W., Olson, Gregory. B., Choudhary, Alok. **Just accepted**. *J. Comp. Chem.* DOI: 10.1002/jcc.25067 (**cover article**)
3. Predictive analytics for crystalline materials: Bulk modulus. Al'ona Furmanchuk, Ankit Agrawal and Alok Choudhary *RSC Adv.*, **2016**, 6, 95246-95251. DOI: 10.1039/C6RA19284J
4. Molecularly Tunable Fluorescent Quantum Defects. Kwon, Hyejin, Furmanchuk, Al'ona, Kim, Mijin, Meany, Brendan, Guo, Yong, Schatz, George, Wang, YuHuang. *J. Am. Chem. Soc.* **2016**, 138, 6878–6885. DOI: 10.1021/jacs.6b03618
5. Multi-step mechanism of carbonization in templated polyacrylonitrile derived fibers: ReaxFF model uncovers origins of graphite alignment. Saha, Biswajit, Furmanchuk, Al'ona, Dzenis, Yuris, Schatz, George C. *Carbon*, **2015**, 94, 694-704. DOI: 10.1016/j.carbon.2015.07.048
6. Molecular Level Engineering of Adhesion in Carbon Nanomaterial Interfaces. M. R. Roenbeck, A. Furmanchuk, Z. An, J. T. Paci, X. Wei, S. T. Nguyen, G. C. Schatz, H. D. Espinosa. *Nano Lett.*, **2015**, 15(7), 4504-4516. DOI: 10.1021/acs.nanolett.5b01011
7. Shear and friction between carbon nanotubes in bundles and yarns. Paci, Jeffrey T., Furmanchuk, Al'ona, Espinosa, Horacio D., Schatz, George C. *Nano Lett.*, **2014**, 14(11), 6138-6147. DOI: 10.1021/nl502210r
8. Inherent carbonaceous impurities on arc-discharge multiwalled carbon nanotubes and their implications for nanoscale interfaces. An, Zhi, Furmanchuk, Al'ona, Ramachandramoorthy, Rajaprakash, Filleter, Tobin, Roenbeck, Michael, Espinosa, Horacio D., Schatz, George C., Nguyen, SonBinh T. *Carbon*, **2014**, 80, 1-11. DOI: 10.1016/j.carbon.2014.07.069
9. Electron induced single strand break and cyclization: a DFT study on the radiosensitization mechanism of the nucleotide of 8-bromoguanine. Chomicz, Lidia, Furmanchuk, Al'ona, Leszczynski, Jerzy, and Rak, Janusz. *Phys. Chem. Chem. Phys.* **2014**, 12, 6568-6574. DOI: 10.1039/C3CP55411B
10. In Situ Scanning Electron Microscope Peeling To Quantify Surface Energy between Multiwalled Carbon Nanotubes and Graphene. Roenbeck, Michael R., Wei, Xiaoding, Beese, Allison M., Naraghi, Mohammad, Furmanchuk, Al'ona, Paci, Jeffrey T., Schatz, George C., and Espinosa, Horacio D. *ACS Nano* **2013**, 8, 124-138, DOI: 10.1021/nn402485n
11. Mechanical properties of silicon nanowires. Furmanchuk, Al'ona, Isayev, Olexandr, Dinadayalane, Tandabany C., Leszczynska, Danuta, Leszczynski, Jerzy. *WILEY Interdisc. Rev.-Comp. Molec. Sci.* **2012**, 2, 817-828, DOI: 10.1002/wcms.1108
12. Morphology and Optical Response of Carbon Nanotubes Functionalized by Conjugated Polymers. Furmanchuk, Al'ona, Leszczynski, Jerzy, Tretiak, Sergei, Kilina, Svetlana V. *J. Phys. Chem. C* **2012**, 116, 6831-6840, DOI: 10.1021/jp211541q

13. Car-Parrinello Molecular Dynamics Simulations of Tensile Tests on Si < 001 > Nanowires. Furmanchuk, Al'ona, Isayev, Olexandr, Dinadayalane, Tandabany C., Leszczynski, Jerzy. *J. Phys. Chem. C* **2011**, 115, 12283-12292, DOI: 10.1021/jp201948g
14. Novel view on the mechanism of water-assisted proton transfer in the DNA bases: bulk water hydration. Furmanchuk, Al'ona, Isayev, Olexandr, Gorb, Leonid, Shishkin, Oleg V., Hovorun, Dmytro M., Leszczynski, Jerzy. *Phys. Chem. Chem. Phys.* **2011**, 13, 4311-4317, DOI: 10.1039/c0cp02177f
15. New insight on structural properties of hydrated nucleic acid bases from ab initio molecular dynamics. Furmanchuk, Alona, Shishkin, Oleg V., Isayev, Olexandr, Gorb, Leonid, Leszczynski, Jerzy. *Phys. Chem. Chem. Phys.* **2010**, 12, 9945-9954, DOI: 10.1039/c002934c
16. Hydration of nucleic acid bases: a Car-Parrinello molecular dynamics approach. Furmanchuk, Al'ona, Isayev, Olexandr, Shishkin, Oleg V., Gorb, Leonid, Leszczynski, Jerzy. *Phys. Chem. Chem. Phys.* **2010**, 12, 3363-3375, DOI: 10.1039/b923930h (**cover article**)
17. Efficient and accurate ab initio prediction of thermodynamic parameters for intermolecular complexes. Isayev, O., Furmanchuk, A., Gorb, L., Leszczynski, J. *Chem. Phys. Lett.* **2008**, 451, 147-152, DOI: 10.1016/j.cplett.2007.11.079
18. Thio- versus oxo-derivatives of DNA bases: theoretical study on possible mutagenic effect of sulfur atom. Furmanchuk, Al'ona, Leszczynski, Jerzy. *J. Sulfur Chem.* **2008**, 29, 401-B17, DOI: 10.1080/17415990802195607
19. Electron Correlated Ab Initio Study of Amino Group Flexibility for Improvement of Molecular Mechanics Simulations on Nucleic Acid Conformations and Interactions. Poltev, V. I., Gonzalez, E., Deriabina, A., Martinez, A., Furmanchuk, A., Gorb, L., Leszczynski, J. *J. Biol. Phys.* **2007**, 33, 499-514, DOI: 10.1007/s10867-008-9091-2
20. Systematic effect of benzo-annulation on oxo-hydroxy tautomerism of heterocyclic compounds. Experimental matrix-isolation and theoretical study. Gerega, Anna, Lapinski, Leszek, Nowak, Maciej J., Furmanchuk, Al'ona, Leszczynski, Jerzy. *J. Phys. Chem. A* **2007**, 111, 4934-4943, DOI: 10.1021/jp070408j
21. Are isolated nucleic acid bases really planar? A Car-Parrinello molecular dynamics study. Isayev, Olexandr, Furmanchuk, Al'ona, Shishkin, Oleg V., Gorb, Leonid, Leszczynski, Jerzy. *J. Phys. Chem. B*, **2007**, 111, 3476-3480, DOI: 10.1021/jp070857j

## B. Software

ThermoEl toolkit. Available at <http://info.eecs.northwestern.edu/ThermoEl>

## C. Abstracts

### *Oral Presentations*

1. MS Annual Meeting & Exhibition, Alloys and Compounds for Thermoelectric and Solar Cell Applications V, Feb. 26 - Mar. 2, 2017. San Diego, CA. Data Science Approaches for Predicting Thermoelectric Properties. A. Furmanchuk, A. Agrawal\*, and A. Choudhary
2. 2016 AIChE Annual Meeting, November 13-18, 2016. San Francisco, CA. Machine Learning for Advancing Discovery of Novel Thermoelectric Materials: ThermoEl. A. Furmanchuk,\* A. Agrawal, J. Saal, J. Doak, G. Olson, and A. Choudhary
3. 250th ACS National Meeting in Boston, Massachusetts to be held August 16-20, 2015. Accurate characterization of nanoscale interfaces. Nature of interactions between inherent carbonaceous clusters and underlying arc-discharge carbon nanotubes. A. Furmanchuk, Z. An, R. Ramachandramoorthy, T. Filleter, M.R. Roenbeck, H.D. Espinosa, G.C. Schatz, S.T. Nguyen.

4. 250th ACS National Meeting .August 16-20, 2015. Boston, MA. Modified graphitic interfaces for effective load transfer in polymer composites. A. Furmanchuk, M.R. Roenbeck, Z. An, J.T. Paci, X. Wei, S.T. Nguyen, G.C. Schatz, H.D. Espinosa
5. 242nd ACS National Meeting, 2011 Denver, CO. Theoretical study of mechanical properties of Si nanowires: At the lower edge of nano. A. Furmanchuk,\* O. Isayev, T. C. Dinadayalane, J. Leszczynski.

### ***Poster Presentations***

1. MS&T'17, Materials Science & Technology 2017 Conference & Exhibition. November 12-16, 2017. San Diego, CA. Data-driven Approaches for Predicting Thermoelectric Properties. Al'ona Furmanchuk, Ankit Agrawal,\* Alok Choudhary.
2. AMIA 2017 Annual Symposium. November 7, 2017. Washington. DC. A Machine Learning-Based Approach for Identifying Atopic Dermatitis in Adults from Electronic Health Records. Erin N. Gustafson,\* Al'ona Furmanchuk,\* Jennifer A. Pacheco, Firas H. Wehbe, Kathryn L. Jackson, Abel N. Kho, William K. Thompson, Jonathan I. Silverberg.
3. AMIA 2017 Annual Symposium. November 7, 2017. Washington. DC. Non-negative Tensor Factorization for Heart Failure Prediction and Novel Subtypes Identification. Yu Deng,\* Faraz S. Ahmad, Robert Chen, Al'ona Furmanchuk, Jimeng Sun, Abel Kho.
4. CHiMAD Annual Meeting. March 23<sup>rd</sup>, 2016. Evanston, IL Data mining tools for thermoelectric materials. Al'ona Furmanchuk,\* Ankit Agrawal, James Saal, Jeff W. Doak, Gregory B Olson, Alok Choudhary.
5. 250th ACS National Meeting in Boston, Massachusetts to be held August 16-20, 2015. Finding the right nanofiller for making highly graphitic carbon nanofibers. What to know about templating mechanism? Al'ona Furmanchuk,\* Biswajit Saha, Yuris A. Dzenis, George C. Schatz.
6. BRI Review: Plasma-Surface Interactions in Reactive Environments December 9, 2014. AFOSR Phillips Technology Institute, NM. Fundamental studies of reactive processes at plasma-surface interfaces. Kelsey M. Stocker,\* Al'ona Furmanchuk,\* George C. Schatz.
7. 2014 Atomic and Molecular Interactions Gordon Research Conference and Seminar. July 13-18, 2014. Easton, MA. Discovering reaction pathways with simulations. Theoretical study of template carbonization in carbon fibers. Biswajit Saha, Al'ona Furmanchuk,\* George C. Schatz.
8. 2014 New Diamond and Nano Carbon Conference. May 25-29, 2014 .Chicago. IL. Surface energy measurements and theory in multi-walled carbon nanotube – graphene systems. Michael R Roenbeck, Xiaoding Wei, Rajaprakash Ramachandramoorthy, Allison M Beese, Mohammad Naraghi, Horacio D Espinosa, Zhi An, SonBinh Nguyen, Alona Furmanchu,\* Jeffrey T Paci, George C Schatz
9. JNCASR-NU Workshop Program on Advanced and Nano-structured Materials. January 14-23, 2013. Bangalor. India. Computational Studies of Carbon nanotubes and graphene structures. Chemistry, optical and mechanical prorteries. Al'ona Furmanchuk,\* Biswajit Saha, George C. Schatz.
10. 20th Conference on Current Trends in Computational Chemistry, 2011 Jackson MS. Applications of Car-Parrinello Molecular Dynamics from Nano to Bio. A. Furmanchuk,\* O. Isayev, T. Dinadayalane, L. Gorb, D. Danuta Leszczynska, J. Leszczynski
11. 242nd ACS National Meeting, 2011 Denver, CO. Prototropic tautomerism in bulk hydration: Is polarizable continuum model really appropriate? A. Furmanchuk,\* O. Isayev, L. Gorb, O. V. Shishkin, D. M. Hovorun, J. Leszczynski

12. 19th Conference on Current Trends in Computational Chemistry, 2010 Jackson MS. Simulations of Tensile Tests in Si <001> Nanowires. A. Furmanchuk, \* O. Isayev, T. Dinadayalane, J. Leszczynski
13. 18th Conference on Current Trends in Computational Chemistry, 2009 Jackson MS. CPMD study of the Young's modulus of nanomaterials. A. Furmanchuk,\* O. Isayev, T. Dinadayalane, and J. Leszczynski
14. Excited State Processes in Electronic and Bio Nanomaterials, 2009 Santa Fe, NM. CPMD study of the Young's modulus of Si nanowires and SWCNTs. A. Furmanchuk,\* O. Isayev, T. Dinadayalane, and J. Leszczynski
15. 237th ACS National Meeting & Exposition, 2009 Salt Lake City, UT. Ab initio Molecular Dynamics Study on the Solute-Solvent Cross-Effects in Nucleic Acid Bases Solutions. A. Furmanchuk,\* O. Isayev, L. Gorb, and J. Leszczynski
16. 237th ACS National Meeting & Exposition, 2009 Salt Lake City, UT. New Protocol for Efficient and Accurate ab initio Prediction of Thermodynamic Parameters. A. Furmanchuk,\* O. Isayev, L. Gorb, and J. Leszczynski
17. 17th Conference on Current Trends in Computational Chemistry, 2008 Jackson MS. Improvement of Molecular Mechanics Force Fields for Nucleic Acids. Ab Initio Based Amino Group Description. A. Furmanchuk,\* V. I. Poltev, E. Gonzalez, A. Deriabina, A. Martinez, L. Gorb, and J. Leszczynski
18. 8th Southern School on Computational Chemistry, 2007 Jackson MS. Novel DNA Bases Analogs. Possible Mutagenic Effect of Sulfur. Al'ona Furmanchuk\* and Jerzy Leszczynski
19. 16th Conference on Current Trends in Computational Chemistry, 2007 Jackson MS. The Hydrogen Bonding of DNA Bases in Aqueous Solution. Ab initio Molecular Dynamics Study. Al'ona Furmanchuk,\* Olexandr Isayev, Leonid Gorb, and Jerzy Leszczynski
20. 15th Conference on Current Trends in Computational Chemistry, 2006 Jackson MS. An *ab Initio* Quantum Mechanical Study of Hydrogen-Bonded Complexes. Al'ona Furmanchuk,\* Olexandr Isayev, Leonid Gorb, and Jerzy Leszczynski
21. 7th Southern School on Computational Chemistry, 2007 Jackson MS. Theoretical Study of Prototropic tautomerism in heteroaromatic compounds. 2(1H)-pyridinone as a model system. Al'ona Furmanchuk,\* Leonid Gorb, and Jerzy Leszczynski
22. 14th Conference on Current Trends in Computational Chemistry, 2005 Jackson MS. Can Gibbs Free Energy for intermolecular complexes be predicted accurately at the MP2 and the DFT levels of theory? Olexandr Isayev, Al'ona Furmanchuk,\* Leonid Gorb, and Jerzy Leszczynski
23. 14th Conference on Current Trends in Computational Chemistry, 2005 Jackson MS. Ab Initio Molecular Dynamics Study: statistical analysis of structural nonrigidity of DNA Bases. Al'ona Furmanchuk,\* Olexandr Isayev, Oleg Sukhanov, Oleg Shishkin, Leonid Gorb, and Jerzy Leszczynski
24. 2nd International Symposium on Recent Advances in Environmental Health Research, 2005 Jackson MS. Molecular Mechanics Computations for Nucleic Acids: ab Initio Accuracy of Guanine Structure. V.I. Poltev, E. Gonzalez, A.S. Deriabina, A. Martinez, Al'ona Furmanchuk,\* L. Gorb, J. Leszczynski.
25. 5th Congress of the International Society for Theoretical Chemical Physics, 2005 New Orleans LA. Structural Nonrigidity of Nucleic Acid Bases. CPMD investigation. Al'ona Furmanchuk,\* Olexandr Isayev, Oleg Sukhanov, Oleg Shishkin, Leonid Gorb, and Jerzy Leszczynski

26. 13th Conference on Current Trends in Computational Chemistry, 2004 Jackson MS. Ab Initio Molecular Dynamics Study on Structural Nonrigidity of Nucleic Acid Bases. Al'ona Furmanchuk,\* Olexandr Isayev, Oleg Sukhanov, Oleg Shishkin, Leonid Gorb, and Jerzy Leszczynski
27. 5th Southern School on Computational Chemistry, 2005 Jackson MS. Some Aspects of Quantum Mechanics Contribution to Improvement of Molecular Mechanics Force Fields. V.I. Poltev, E. Gonzalez, A. Deriabina , L. Lozano, A. Martinez, A. Furmanchuk,\* T. Robinson, L. Gorb, J. Leszczynski
28. 4th Southern School on Computational Chemistry, 2004 Orange Beach AL. Combined ab initio molecular dynamics and quantum-chemical study of selected chemical processes of biological importance. L.Gorb, O. S. Sukhanov, O. Isayev, A. Furmanchuk,\* I, Tunon, M.F. Ruiz-Lopez, O. V. Shishkin and J. Leszczynski
29. 12th Conference on Current Trends in Computational Chemistry, 2003 Jackson MS. Theoretical Investigation of 3-Methyl-Cytosine Hydration. Al'ona Furmanchuk,\* Olexandr Isayev, Leonid Gorb and Jerzy Leszczynski