Mahdi Davari

Institute for Advanced Computational Science, Center for Materials by Design, and Department of Geosciences.
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Experience

2018 - Now **Postdoctoral Research Fellow** Stony Brook University, NY
Mentor: Artem R. Oganov , John B. Parise
Research Focus: Crystal structure prediction, superconductivity, deep interior of the Earth and high pressure physics/chemistry.

2013 - 2017 **Graduate Research Assistant** Stony Brook University, NY
Ab initio design of inorganic materials with desired properties. Novel compounds under high pressure conditions (borides, hydrides, oxynitrides, etc). Search for novel superconducting materials, using evolutionary algorithm, and developing new functionalities for efficiently searching the energy landscape of materials. Prediction of novel hydrides with high-temperature superconductivity. High-throughput materials discovery with focus on materials for energy generation and storage applications.

2014 - Now **Scientific Software Developer** Center for Materials by Design, NY
Design and development of crystal structure prediction algorithms implemented in USPEX code (used by over 4000 researchers worldwide). Implementing a descriptor of structure (fingerprint function), enabling quantification of energy landscapes of 2D materials. Developing a method for two-parameter optimizations, enabling the search for materials with desired properties along with the stability.

2014 - Now **HPC System Administrator and webmaster** Center for Materials by Design, NY
Design, development and management of USPEX website and user database on SQL databases. Configuring and managing high performance computing cluster on Red Hat/Debian platform.

2013 - 2014 **Graduate Teaching Assistant** Stony Brook University, NY
Performed academic tutoring in GEO 112: Physical Geology Lab. Provided assistance to professors and students in GEO 105: Energy Resources for the 21st Century and GEO102: The Earth.

2011 - 2012 **Graduate Teaching Assistant** Isfahan University of Technology, Iran
Lab instructor and lecturer of 4 Physics Labs (undergraduate level).

Technological Skills

- **Operating System:** using and administrating Linux, Mac and Windows
- **Computational Software:** Python, MATLAB, R and working knowledge of C++
- **Typesetting:** LaTeX, LibreOffice, Microsoft office, iWork
- **Graphics Software:** Adobe Photoshop, Adobe Illustrator, Affinity Designer, Gimp
- **Scientific Packages:** USPEX, VASP, Quantum-Espresso, GULP, FHI-aims and Octopus
- **Other:** Xcode, JetBrain suite, SVN, Git, SQL and GitKraken

Research Interests

- High-throughput materials design
- Crystal structure predictions
- Photocatalyst materials for water splitting (oxynitrides – energy materials)
- Superconductivity (hydrides - borides)
- Transition metal compounds
- Developing methods in searching energy landscapes of crystals
- Pressure induced stability and high pressure physics/chemistry

Education

2013 - 2017 **Ph.D. in Computational Chemistry/Physics** Stony Brook University, NY, USA
Geosciences Dep., Supervisors Prof. Artem R. Oganov, Prof. John B. Parise
Main subjects: Computational materials discovery, crystallography, materials properties, superconductivity, energy materials and high pressure physics/chemistry.
Title of the Thesis: "Novel superconducting phases of materials under pressure by Evolutionary Algorithm USPEX".

2010 - 2012 **M.Sc. in Condensed Matter Physics** Isfahan University of Technology, Iran
Physics Department., Supervisor Dr. Mojtaba Alaei
Main subjects: Computational physics, optical properties and TDDFT.
Title of the Thesis: "Optical properties of tungsten oxide clusters $(WO_3)_n$ n=1-6 with time dependent density functional theory (TDDFT)".

2005 - 2010 **B.Sc. in Condensed Matter Physics** University of Isfahan, Iran
Physics Department

Publications

Book Chapter

1. Computational Materials Discovery, Royal Society of Chemistry; (November, 2018) DOI: 10.1039/9781788010122

Peer review papers (14+ papers in total, 70+ citations since 2016)

1. **M. M. Davari Esfahani**, Z. Wang, A. R. Oganov, H. Dong, Q. Zhu, S. Wang, M. S. Rakitin, and X.-F. Zhou, "Superconductivity of novel tin hydrides (Sn_nH_m) under pressure," *Sci. Rep.*, vol. **6**, 22873, 2016.
2. **M. M. Davari Esfahani**, A.R. Oganov, H. Niu and J. Zhang "Superconductivity and unexpected chemistry of germanium hydrides under high pressure" *Phys. Rev. B*, **95** (13), 134506, 2017.
3. **M. M. Davari Esfahani**, Q. Zhu, H. Dong, A. R. Oganov, S. Wang, M. S. Rakitin, and X.-F. Zhou "Novel magnesium borides and their superconductivity," *Phys. Chem. Chem. Phys.*, **19**, 14486-14494, 2017.
4. A. James, **M. M. Davari Esfahani**, W. Woerner, A. Sinclair, L. Ehm, A. R. Oganov, and J. B. Parise. "Theoretical and Experimental Investigations into Novel Oxynitride Discovery in the GaN-TiO_2 System at High Pressure," *Crystals.*, vol. **8**, no. 2, 2018.
5. N. P. Salke, **M. M. Davari Esfahani**, Y. Zhang, I. A. Kruglov, J. Zhou, Y. Wang, E. Greenberg, V. B. Prakapenka, A. R. Oganov, J-F. Lin. "Synthesis of clathrate cerium superhydride CeH9 at 80 GPa with anomalously short H-H distance," *Submitted to Nature Materials*, 2018.

6. N. P. Salke, **M. M. Davari Esfahani**, Y. Zhang, I. A. Kruglov, J. Zhou, A. R. Oganov, J-F. Lin, "Synthesis and prediction of dysprosium hydride at high pressure," *under preparation*, 2018.
7. M. S. Rakitin, A. R. Oganov, H. Niu, **M. M. Davari Esfahani**, X.-F. Zhou, G.-R. Qian, and V. L. Solozhenko, "A novel phase of beryllium fluoride at high pressure," *Phys. Chem. Chem. Phys.*, vol. **17**, no. 39, pp. 26283–26288, 2015.
8. I. A. Kruglov, D. V Semenok, R. Szczęśniak, **M. M. Davari Esfahani**, A. G Kvashnin, A. R. Oganov. "Superconductivity in LaH_{10} : a new twist of the story" *arXiv preprint* arXiv:1810.01113 (2018).
9. Y. Naleem and **M. M. Davari Esfahani**, "Prediction of martensitic phase transformation in alkaline-earth halofluoride scintillating materials under high pressure," *Submitted to Phys. Rev. B*, 2018.
10. S. Wang, A. R. Oganov, G. Qian, Q. Zhu, H. Dong, X. Dong, and **M. M. Davari Esfahani**, "Novel superhard B-C-O phases predicted from first principles," *Phys. Chem. Chem. Phys.*, vol. **18**, 3, 1859–1863, 2016.
11. H. Dong, A. R. Oganov, Q. Wang, S.-N. Wang, Z. Wang, J. Zhang, **M. M. Davari Esfahani**, X.-F. Zhou, F. Wu, and Q. Zhu, "Prediction of a new ground state of superhard compound B_6O at ambient conditions," *Sci. Rep.*, **6**, 31288, 2016.
12. J. Zhang, A. R. Oganov, X. Li, **M. M. Davari Esfahani**, and H. Dong "First-principles investigation of Zr-O compounds, their crystal structures, and mechanical properties", *J. Appl. Phys.* **121**, 155104, 2017.
13. I. Kruglov, R. Akashi, S. Yoshikawa, A. R. Oganov, and **M. M. Davari Esfahani**, "Refined phase diagram of the H-S system with high-T_c superconductivity", *Phys. Rev. B*, **96** (22), 220101, 2017.
14. H. Dong, A. R. Oganov, V. Brazhkin, Q. Wang, S.-N. Wang, Z. Wang, J. Zhang, **M. M. Davari Esfahani**, X.-F. Zhou, F. Wu, and Q. Zhu, "Boron oxides under pressure: Prediction of the hardest oxides", *Phys. Rev. B*, 2018.
15. **M. M. Davari Esfahani**, M. Alaei, "Optical properties of tungsten-oxide clusters with time-dependent density functional theory" *National condensed matter conference, Shahrood, 2012*.

Invited/contributed talks

- American Chemical Society National Meeting, Boston, MA, 2018
- Materials Research Society Spring Meeting, Phoenix, AZ, 2017
- Symposium: Computational Crystallography, New York University, NY, 2017
- Nanomaterials: Computation, Theory, and Experiment, TSRC, Telluride, CO, 2017
- American Chemical Society March Meeting, San Diego, CA, 2016

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December 3, 2018

M. Mahdi Davari Esfahani