MICHAEL ASHTON

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Summary

I am a motivated learner who loves engaging with others on a team. I hope to use my experience and passion for computational materials research and software design to make real progress toward designing and discovering useful materials properties.

Skills

DFT, Python, C++, Git, Django, Jekyll, Linux, MongoDB, CI, HTML/CSS, javascript

Education and Research

Postdoc - Max Planck Institute for Iron Research

Düsseldorf, Germany (Nov. 2017-Present)

As part of the Defect Chemistry and Spectroscopy group, I designed and performed first-principles investigations of atomic bond breaking under extreme electric fields.

Doctor of Philosophy (Materials Science)

University of Florida, April 2017

GPA: 3.95/4

Advisors: Dr. Richard Hennig and Dr. Susan Sinnott

Thesis:

Computational Methods for the Discovery and Characterization of Two-Dimensional Materials

Bachelor of Science (Materials Science)

University of Florida, May 2013

GPA: 3.88/4, graduated Summa cum Laude

Concentration in metallurgy

Selected Publications (full list available on Google Scholar)

1. **Ashton, M.**, Mishra, A., Neugebauer, J., and Freysoldt, C., *Ab Initio* Description of Bond-Breaking in Large Electric Fields, *Phys. Rev. Lett.* 2020 https://doi.org/10.1103/PhysRevLett.124.176801

2. **Ashton, M.**, Mathew, K., Suntevich, J., Freysoldt, C., Sinnott, S. B., and Hennig, R. G., Predicting the Electrochemical Synthesis of 2D Materials from First-Principles, *J. Phys. Chem. C* 2019 https://doi.org/10.1021/acs.jpcc.8b10802

3. **Ashton, M.**, Gluhovic, D., Sinnott, S. B., Guo, J., Stewart, D. A., and Hennig, R. G., Two-Dimensional Half-Metals with Large Spin Gaps, *Nano Lett.* 2017 https://doi.org/10.1021/acs.nanolett.7b01367

4. **Ashton, M.**, Paul, J., Sinnott, S. B, and Hennig, R. G., Topology-Scaling Identification of Layered Solids and Stable Exfoliated Monolayers, *Phys. Rev. Lett.* 2017 https://doi.org/10.1103/PhysRevLett.118.106101

5. Gault, B., Saxey, D. W., **Ashton, M.**, Sinnott, S. B., Chiaramonti, A. N., Moody, M. P., and Schrieber, D. K., Behavior of Molecules and Molecular Ions Near a Field Emitter, *New J. Phys*. 2016 https://dx.doi.org/10.1088/1367-2630/18/3/033031

Awards and Other Work

Alexander von Humboldt award for Postdoctoral Researchers (2019)

pyrho (real-space DFT package in python)

https://github.com/ashtonmv/pyrho

- Creator and lead developer
- Used code to introduce several masters/PhD students to DFT fundamentals

pyiron (python framework for materials simulation)

https://pyiron.org

- Developer, designed input class for simulations & calculations used throughout codebase
- Website creator and maintainer

SPHInX (C++ DFT package)

https://sxrepo.mpie.de

- Developed van der Waals and Hirschfeld charge partitioning submodules

Materialsweb/MPInterfaces (2D Materials database)

https://materialsweb.org

- Designed and developed the website and online database
- Core developer for MPInterfaces (the python backend for generating and analyzing materials data)

References

- Professor Susan B. Sinnott, Dept. Head and Prof. of Materials Science, Penn State University
  sinnott@matse.psu.edu

- Professor Richard G. Hennig, Prof. of Materials Science, University of Florida
  rhennig@mse.ufl.edu

- Dr. Christoph Freysoldt, Group Leader, Max Planck Institute for Iron Research
  freysoldt@mpie.de