SI2-SSI Collaborative Research: A Computational Materials Data and Design Environment

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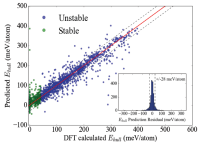
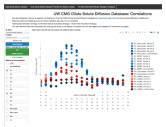
Developed tools/data for computational materials design:

The Materials Simulation Toolkit (MAST) for high-throughput defect and diffusion modeling[1]

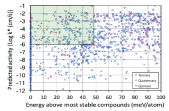


A Machine Learning extension (MAST-ML) to rapidly generate machine learning models from materials data[2].

Online defect and diffusion analysis apps on MaterialsHub[3].

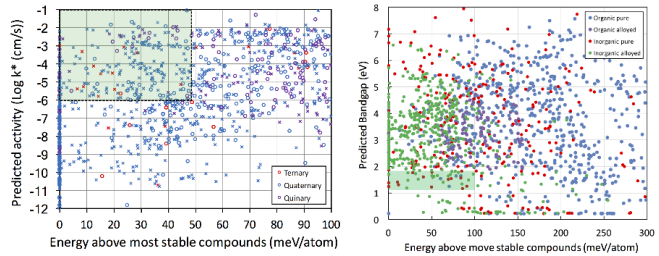


The world's largest computed and machine learning enhanced diffusion database with easy online search[4].

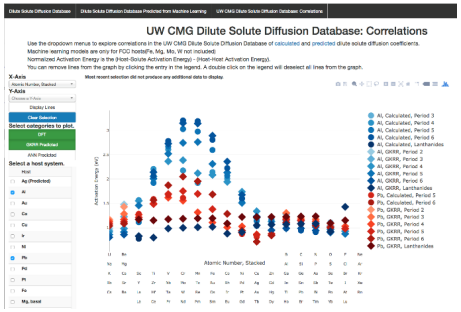


Valuable research results using these tools and data, e.g. new fuel cell materials[5].

Workforce training through the *Informatics Skunkworks*, an undergraduate materials informatics group[6].



New materials for fuel and solar cells.



Database of of diffusion coefficients.

WISCONSIN innovation awards Finalist

50+ undergraduates in Skunkworks

[1] T. Mayeshiba, et al. Comp. Mat. Sci. '17; pypi.python.org/pypi/MAST ; [2] github.com/uw-cmg/MAST-ML ; [3] materialshub.org ; [4] diffusiondata.materialshub.org ; Wu, et al., *Scientific Data* '16 and *Comp. Mat. Sci.* '17; [5] E.g., Jacobs, et al., *Advanced Energy Materials* '18 ; [6] skunkworks.engr.wisc.edu/