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"Matminer and Automatminer: Software Tools for Accelerating Materials Discovery with Machine Learning."

Abstract: In this talk we present matminer (github.com/hackingmaterials/matminer), an open-source Python-based software tool for data analytics and machine learning (ML) in materials science. Matminer hosts a growing repository of 60+ routines for robustly generating ML descriptors for crystal structures, chemical compositions, and electronic bandstructures. Matminer also contains infrastructure for easily retrieving community datasets used in peer-reviewed studies and for generating new datasets from online databases such as the Materials Project, the Materials Data Facility, AFLOW, and more. Using these resources, matminer enables the accelerated deployment and comparison of machine learning models for materials discovery. Next, we present Automatminer, a completely automatic ML package for materials property prediction built on top of Matminer. Finally, we compare Automatminer's results with recent human-optimized models and state-of-the-art crystal-graph networks in predicting electronic, elastic, optical, vibrational, and thermodynamic properties across a variety of computational and experimental datasets. Authors: Alex Dunn, Qi Wang, Alireza Faghaninia, Alex Ganose, and Anubhav Jain.