

Abstract Submitted
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Learning targeted materials properties from data TURAB LOOKMAN, PRASANNA V BALACHANDRAN, XUE DEZHEN, JAMES THEILER, JOHN HOGDEN, Los Alamos Natl Lab — We compare several strategies using a data set of 223 M₂AX family of compounds for which the elastic properties [bulk (B), shear (G), and Young's (E) modulus] have been computed using density functional theory. The strategy is decomposed into two steps: a *regressor* is trained to predict elastic properties in terms of elementary orbital radii of the individual components of the materials; and a *selector* uses these predictions to choose the next material to investigate. The ultimate goal is to obtain a material with desired elastic properties. We examine how the choice of data set size, regressor and selector impact the results.

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