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Universal Fragment Descriptors for Predicting Electronic and Mechanical Properties of Inorganic Crystals COREY OSES, Duke Univ, OLEXANDR ISAYEV, Univ of North Carolina, Chapel Hill, CORMAC TOHER, STEFANO CURTAROLO, Duke Univ, ALEXANDER TROPSHA, Univ of North Carolina, Chapel Hill — Historically, materials discovery is driven by a laborious trial-and-error process. The growth of materials databases and emerging informatics approaches finally offer the opportunity to transform this practice into data- and knowledge-driven rational design—accelerating discovery of novel materials exhibiting desired properties. By using data from the AFLOW repository for high-throughput, *ab-initio* calculations, we have generated Quantitative Materials Structure-Property Relationship (QMSPR) models to predict critical materials properties, including the metal/insulator classification, band gap energy, and bulk modulus. The prediction accuracy obtained with these QMSPR models approaches training data for virtually any stoichiometric inorganic crystalline material. We attribute the success and universality of these models to the construction of new materials descriptors—referred to as the universal Property-Labeled Material Fragments (PLMF). This representation affords straightforward model interpretation in terms of simple heuristic design rules that could guide rational materials design. This proof-of-concept study demonstrates the power of materials informatics to dramatically accelerate the search for new materials.

Corey Oses
Duke Univ

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