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A comprehensive polymer dataset for accelerated property prediction and design HUAN TRAN, ARUN KUMAR MANNODI-KANAKKITHODI, CHIHO KIM, University of Connecticut, VINIT SHARMA, Oak Ridge National Laboratory, GHANSHYAM OILANIA, Los Alamos National Laboratory, RAMPI RAMPRASAD, University of Connecticut — Emerging computation- and data-driven approaches are particularly useful for rationally designing materials with targeted properties. In principle, these approaches rely on identifying structure-property relationships by learning from a dataset of sufficiently large number of relevant materials. The learned information can then be used to rapidly predict the properties of materials not already in the dataset, thus accelerating the design of materials with preferable properties. Here, we report the development of a dataset of 1,065 polymers and related materials, which is available at http://khazana.uconn.edu/. This dataset is uniformly prepared using first-principles calculations with structures obtained either from other sources or by using structure search methods. Because the immediate target of this work is to assist the design of high dielectric constant polymers, it is initially designed to include the optimized structures, atomization energies, band gaps, and dielectric constants. The dataset will be progressively expanded by accumulating new materials and including additional properties calculated for the optimized structures provided. We discuss some information "learned" from the dataset and suggest that it may be used as the playground for further data-mining work.

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