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Rational Co-Design of Polymer Dielectrics for Energy Storage

ARUN MANNODI-KANAKKITHODI, HUAN TRAN, University of Connecticut, GHANSHYAM PILANIA, TURAB LOOKMAN, Los Alamos National Laboratory, RAMPI RAMPRASAD, University of Connecticut — While intuition-driven experiments and serendipity have guided traditional materials discovery, computational strategies have become increasingly important and a powerful complement to experiments in modern day materials research. With the example of polymer dielectrics for electrostatic energy storage applications, we demonstrate how a rational co-design approach—involving synergies between high-throughput computational screening and experimental synthesis and testing—can be harnessed for quick and efficient discovery. We highlight recent co-design efforts that can potentially lead to replacement of present-day "standard" polymer dielectrics (such as biaxially oriented polypropylene) not only by new organic polymer candidates within known generic polymer subclasses (e.g., polyurea, polythiourea, polyimide), but also by organometallic polymers, a hitherto untapped but promising chemical subspace. We also discuss the utilization of vast computational data (generated in the aforementioned process) towards the development of statistical learning models for relevant properties of dielectric polymers, which can further accelerate the guidance to experiments and thus the successful discovery of new materials.

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