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The Harvard Clean Energy Project: High-throughput screening of organic photovoltaic materials using cheminformatics, machine learning, and pattern recognition ROBERTO OLIVARES-AMAYA, JOHANNES HACHMANN, Harvard University, CARLOS AMADOR-BEDOLLA, Universidad Nacional Autónoma de México, AIDAN DALY, ADRIAN JINICH, SULE ATAHAN-EVRENK, Harvard University, SERGIO BOIXO, University of Southern California, ALÁN ASPURU-GUZIK, Harvard University — Organic photovoltaic devices have emerged as competitors to silicon-based solar cells, currently reaching efficiencies of over 9% and offering desirable properties for manufacturing and installation. We study conjugated donor polymers for high-efficiency bulk-heterojunction photovoltaic devices with a molecular library motivated by experimental feasibility. We use quantum mechanics and a distributed computing approach to explore this vast molecular space. We will detail the screening approach starting from the generation of the molecular library, which can be easily extended to other kinds of molecular systems. We will describe the screening method for these materials which ranges from descriptor models, ubiquitous in the drug discovery community, to eventually reaching first principles quantum chemistry methods. We will present results on the statistical analysis, based principally on machine learning, specifically partial least squares and Gaussian processes. Alongside, clustering methods and the use of the hypergeometric distribution reveal moieties important for the donor materials and allow us to quantify structure-property relationships. These efforts enable us to accelerate materials discovery in organic photovoltaics through our collaboration with experimental groups.

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