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Accelerated Discovery of Organic Photovoltaic Materials through Atomic Scale Simulation

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Organic photovoltaic (OPV) devices are under widespread development to complement or displace existing inorganic solar cells. The materials in these devices are selected or designed according to their intrinsic and extrinsic electronic properties with concern for efficient charge injection and transport, and desired stability and light adsorption characteristics. The chemical design space for OPV materials is enormous and there is need for the development of computational approaches to help identify the most promising solutions for experimental development. In this presentation we will present an overview of simulation approaches available to efficiently screen libraries of potential OPV materials; including first-principles prediction of key intrinsic properties, classical simulation of amorphous morphology, and quantum-mechanics evaluation of electron coupling for molecules in the condensed phase.

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