Computational Design of Organic Solar Cells: Genetic Algorithm-Driven Inverse Design

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Organic solar cells offer the promise of the incredibly tailorability of synthetic chemistry to control properties, mixed with the potential of low-cost electrical generation. Progress has been slowed by the vast "design space" of molecules and the complicated interplay of properties, buried interfaces, and trial-and-error film deposition techniques. We will outline the current state-of-the-art of both experiment and theory, focusing on the rapid computational design of simple optical properties (e.g., band gap) and energy levels (oxidation and reduction potentials) and charge transport simulations. Our lab has pioneered the use of genetic algorithms and multi-tier screening to efficiently find interesting targets. We also accurately treat transport of delocalized charges through 2D and 3D films and are using genetic algorithm and image processing techniques to find optimal film morphology and device structures.