Designing Optoelectronic Materials Using Genetic Optimization: From Small Emitters to Large Interfaces

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Several atomistic simulation workflows have been assembled into a knowledge discovery interface that can be used to streamline the design of materials with specific optoelectronic- and/or structure-based properties. The optoelectronics component uses Jaguar, Schrödinger's quantum chemistry package, with a customizable level of accuracy, to calculate properties like redox potentials, reorganization energies, and spin-splitting energies as well as absorption spectra and the S1-T1 gap necessary for investigating thermally activated delayed fluorescence (TADF). Emission and conduction layers and interfaces built from organic molecules, metal complexes, polymers, and/or crystalline materials are simulated using Desmond, D. E. Shaw Research's molecular dynamics package. An efficient supervised learning protocol can then be used to drive the optoelectronics component using genetic optimization. Candidate solutions can be prepared from a database or by using interactive, alchemical, or reaction channel enumeration. A state-of-the-art GUI allows for automatic and interactive analysis of a huge number of results complete with several plotting options, evolution visualization, absorption spectra, etc. Several details and some interesting applications will be presented.