

[Donor-acceptor copolymers for intramolecular singlet fission](#)

This interactive dataset contains 2944 synthetically feasible donor-acceptor systems screened for intramolecular singlet fission capability. The computed properties of the dimer (excitation energies, singlet-triplet energy splitting, excited state character, dihedral angle between units) and of the constituent monomers (frontier molecular orbital energies, excitation energies, singlet-triplet energy splitting) are provided. The reader is invited to explore the interplay of these properties by choosing the variables that are represented in the x, y, z and color axes. Clicking on a point in the plot provides the DFT-optimized geometry and relevant properties for that dimer alongside its SMILES string, which allows for rapid transferability of the structure to other chemistry software.

Further information on methods, results and the full dataset are given in the references shown below.

[Materials Cloud](#)

[Explore the full provenance](#)