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New way of polymer design for organic solar cells using the quinoid structure NICOLAS BERUBE, JOSIANE GAUDREAU, MICHEL COTE, Universite de Montreal — Research in organic photovoltaic applications are receiving a great interest as they offer an environmentally clean and low-cost solution to the world's rising energy needs. Controlling the device's active polymer optical bandgap is an important step that affects its absorption of the solar spectrum, and ultimately, its power conversion efficiency. The use of fused heterocycles that favors the polymer's quinoid structure has been a known method to lower the bandgap, for example, with isothianapthene, but there is a lack of quantifiable data on this effect. Density functional theory (DFT) calculations were done on over 60 polymers with bandgaps between 0.5 eV and 4 eV. They clearly show that low bandgaps are observed in copolymers that carefully stands between their quinoid and aromatic structures. Such balance can be obtained by mixing monomer units with quinoid characteristics with aromatic ones. Time-dependant DFT results also links low bandgaps with lower reorganization energy, which means that polymers with this structural form could possess higher charge mobilities. This link between the geometrical structure and the bandgap is compatible with a vast variety of polymers and is more convincing than the commonly used donor-acceptor method of polymer design.

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