Delocalized exciton formation in C60 linear molecular aggregates

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Abstract: Organic semiconducting materials containing C60 molecules are efficient acceptors for planar perovskite solar cells. In this work, we theoretically investigate the optical and excitonic properties of C60 linear molecular aggregates (composed of 1 to 7 C60 molecules) *via* the real-time-propagation rt-TDDFT technique. In the case of a single C60 molecule, the photoabsorption peaks are dominated by localized molecular excitons. We furthermore demonstrate that, in the case of linear molecular aggregates, the photoabsorption peaks are contributed by localized molecular excitons, charge transfer excitons, and Wannier-like delocalized excitons. This result is different to the accepted theory that only localized molecular excitons or charge transfer excitons can be produced in organic semiconducting materials. This work provides additional insights into the exciton formation in C60 molecular aggregates and may help in the rational design of efficient solar cells.