Theoretical Study of Carbazole Dimers: Does Carbazole Form an Excimer That Undermines the Performance of Organic Light Emitting Diodes?

Kyungeon Lee[1] and Dongwook Kim[1]

[1]Kyonggi University

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Abstract

Carbazole (Cz) dimers in various cofacial conformations, including staggered (*Stg*), *anti*, and *syn*, were explored by means of ab initio calculations at SOS-MP2, SOS-CIS(D_0), and additional coupled cluster calculation levels. As in other π-conjugated molecules, strong Cz excimers form in the *syn* conformation in both the S_1 and T_1 states, leading to significantly reduced optical excitation energies, whereas the dimers in the *Stg* and *anti* conformations, upon excitation, remain as simple excited dimers, showing similar optical energy gaps to that of the monomer. Being far more stable in the ground state, however, the *Stg* dimer turned out to be nearly isoenergetic to the *syn* dimer in the S_1 state, and even more stable in the T_1 state. In addition, a considerable potential energy barrier between the *syn* and *Stg* dimers was found in the calculated S_1-state potential energy surface. Given that the ground-state intermolecular interactions are expected to govern the dimer conformations of Cz-based materials in the solid-state films of organic electronics, these results strongly demonstrate that the electronic excitation of Cz dimers do not necessarily lead to the strong excimer formation, unless Cz molecules were forced to be arranged in the *syn* conformation.

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