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Theoretical investigation of perylene dimers and excimers and their signatures in X-ray diffraction

The structures of the ground and excimer states of perylene pairs are calculated [using density functional theory (DFT) and time-dependent DFT techniques] in a free as well as a crystal environment, and their spectroscopic properties are studied for the most stable configurations. The vertical transition energies for the absorption and emission bands are obtained, and they are in good agreement with experimental data. In these calculations, up to six excited states are considered. With the calculated structures of the ground and excimer states, the scattering factors are analyzed as a function of the concentration of excimers in a crystal. The intensity of the 110, 005, and 0 10 0 reflections are found to be fairly sensitive to the presence of excimers in the crystal. The finite (nanosecond) lifetime of the excimer may make it possible to observe this state using time-resolved X-ray diffraction techniques.

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