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Computational Analysis of Mechano-Sensitive Chiral Luminescence in Organic Materials: a TDDFT Approach

Difluoro-boron β-diketonate (DFB) amide derivatives, such as (S)-DFB-PhEt-amide and (S)-DFB-Hex-amide, have emerged as promising candidates for applications in optoelectronics and sensing due to their mechano-responsive chiroptical properties. Despite their potential, the molecular origins of these behaviours are still not fully understood. This work presents a detailed computational study designed to explore these systems, supported by comparison with experimental observations [1]. We employed Density Functional Theory (DFT) [2] and Time-Dependent DFT (TDDFT) [3] to investigate the crystal packing, excited-state electronic transitions, and chiroptical signatures of these materials. Results show that the accuracy of predicted geometries depends strongly on the chosen functional and basis set. TDDFT calculations reproduced UV/Vis and Circular Dichroism (CD) spectra in good agreement with experimental data [1]. Structural reorganization upon excitation directly influences chiral emission [4], positioning these systems as relevant prototypes for CPL-active material design [5].

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