Abstract Submitted
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Frenkel-Charge-Transfer exciton intermixing theory for molecular crystals with two isolated Frenkel exciton states.[1] IGOR BONDAREV, ADRIAN POPESCU, North Carolina Central University — We develop an analytical theory for the intra-intermolecular exciton intermixing in periodic 1D chains of planar organic molecules with two isolated low-lying Frenkel exciton states, typical of copper phthalocyanine (CuPc) and other transition metal phthalocyanine molecules[1,2]. We formulate the Hamiltonian and use the exact Bogoliubov diagonalization procedure to derive the eigen energy spectrum for the two lowest intramolecular Frenkel excitons coupled to the intermolecular charge transfer (CT) exciton state. By comparing our theoretical spectrum with available experimental CuPc absorption data, we obtain the parameters of the Frenkel-CT exciton intermixing in CuPc thin films. The two Frenkel exciton states here are spaced apart by 0.26 eV, and the charge transfer exciton state is 50 meV above the lowest Frenkel exciton. Both Frenkel excitons are strongly mixed with the CT exciton, showing the coupling constant 0.17 eV in agreement with earlier electron transport experiments[3]. Our results can be used for the proper interpretation of the physical properties of crystalline phthalocyanines. – [1]J.H.Sharp, M.Abkowitz, J. Phys. Chem. 77, 477 (1973); [2]L.Edwards, M.Gouterman, J. Mol. Spectr. 33, 292 (1970); [3]I.G.Hill at al., Chem. Phys. Lett. 327, 181 (2000).

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