Electronic excitations of C 60 aggregates

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Excitation properties of the isolated C 60 and (C 60) N model clusters (N = 2, 3, 4, 6 and 13) are studied using an a priori parameterized and self-consistent Hamiltonian, the Complete Neglect of Differential Overlap considering the l azimuthal quantum number method. This method properly describes electron excitations of the isolated C 60 after the configuration interaction of singles (CIS) procedure, when those are compared with experimental data in n-hexane solution and in a molecular beam. Geometry models of (C 60) N clusters to model the effect of aggregation were obtained from the fullerene fcc crystal. Some peaks in the low energy edge of the absorption spectrum appear corresponding to clustering effects, as well as small increases of bandwidths in the strong bands at the UV region. An analysis of the theoretical absorption spectrum for dimer models has been carried out, taking into account the influence of the distance between fullerene centers. The density of states of CIS for