Interacting Electrons in SWCNT with sp^3 defects Described by Slater Determinant

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Carbon nanotubes with optically active sp^3 defects have interesting signatures of electron-electron interaction. These effects are explored by focusing on 2 mid-gap electrons trapped in two sp^3 defects. For a focused exploration one reduces dimension of the problem as follows: DFT modeling of aniline-functionalized (11,0) CNTs with periodic boundary conditions provide data for the 3D Kohn-Sham potential, which is imported and projected onto 1D potentials. Here one uses a framework of 1D one electron potential for a simplistic assessing of e-e interaction by exploring two electrons filling this 1D potential. Using a specific MATLAB script, one observes the variation in energies for the eigenstates, values, and energy as the defects are placed at increasing distance. It was shown that as the distance between the defects increased, the energy potential decreased, to account for electron-electron interaction, the lowest eigenstates of these 1D potentials were combined into a Slater determinant to account for the anti-symmetry and to avoid the infinite value of the coulomb interaction. First, one considers a Slater determinant composed of the eigenstates i=1, j=2. Second, one considers a Slater determinant of an excited state i=1, j=4. Properties of these Slater Determinants were explored as function of distance between defects in the model.

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