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Strong Correlation Effects in Fullerene Molecules and Solids

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Fullerenes (C₂₀, C₃₆, C₆₀) are a family of Carbon cage molecules that have exactly twelve pentagons. The most famous Fullerene is C₆₀ (“bucky ball”), which when being doped with three electrons per molecule will exhibit superconductivity. Here we describe electronic structures of these molecules with a tight-binding Hubbard model and solve the model with quantum Monte Carlo simulations and exact diagonalization method. We will show how the electronic correlation gets stronger as the molecule becomes more curved, how the strong electronic correlations change the Huckel molecular energy levels, and how we compare the single-particle excitation spectrum for the C₆₀ molecular solid to the photoemission experiments.