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Density functional calculation of superatomic molecular orbitals in C60: First truly converged results on a real grid mesh[1] KYLE DRAKE, JASON BONACUM, GUO-PING ZHANG, Indiana State University — The molecular structure of Buckminster fullerene (C60) allows for electron delocalization in all of the pi-bonding electrons of the molecule. This coupled with the symmetry of the molecule allows for the formation of super-atomic molecular orbitals (SAMOs) similar to those observed in aluminum clusters. The SAMOs behave as if the molecule that they belong to is a single atom. We compute the eigenstates of C60 computationally using density functional theory (DFT) and a grid mesh. Using larger radii also allows us to accurately describe SAMOs and test the convergence of our data. The results are interesting because for the first time, we can show the true converged super atomic orbitals in C60.

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