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Superatomic Molecular Orbitals of C60: First-Principles calculation JASON BONACUM, GUO-PING ZHANG, KYLE DRAKE, Indiana State Univ — The molecular structure of buckminsterfullerene or C60 allows for highly delocalized orbitals, but they are not like a planewave, which is completely delocated. Instead they form super atomic molecular orbitals (SAMO). These SAMO are like regular atomic orbitals, but the molecule now acts as a single atom. This implies that SAMO should follow trends similar to that of regular atomic orbitals. Using density functional theory in a real grid mesh, we computed these SAMO of C60. We found that the trend in the orbitals corresponding to these eigenstates can then be compared to the valence electron orbital trends on the periodic table. This information is useful for determining the properties of C60 that are a result the SAMO, and these properties are important in the applying C60 as building blocks in the field of nanoscience.

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