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Super Atomic Molecular Orbitals of Variably Protonated Symmetric Molecules[1] TANNER LATTA, KYLE DRAKE, G.P. ZHANG, Indiana State Univ — The molecular structure of symmetric molecules creates conducive conditions for delocalized orbitals. The π bonding delocalizes the valence electrons away from the individual molecules. These delocalized valence electrons allow the symmetric molecules to adapt the characteristics analogous to that of an individual atom, creating Super Atomic Molecular Orbitals, SAMOs. The symmetric molecule is then comparable to that of an individual atom with its regular atomic orbitals. When these symmetric molecules are protonated in any form, there are notable changes in the shapes of the Super Atomic Molecular Orbitals. We use the Density Functional Theory with a grid mesh method to compute the wavefunctions of those SAMOs. Then we examine the Rydberg States of these symmetric molecules through the calculated Eigenstates, and find an important trend in the filling of the SAMOs as well as relationships between variably protonated symmetric molecules. This is potentially very useful to understanding the photovoltaic effect in the fullerene-based solar cells.

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