

Abstract Submitted
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DFT study on the charge density shift bucky-ferrocene vs. bucky-ruthenocene TUNNA BARUAH, RAJENDRA ZOPE¹, University of Texas at El Paso, MARK PEDERSON, Naval Research Laboratory — Iron and ruthenium atoms have similar valence electron configurations. Ferrocene and ruthenocene are stable metallocenes that satisfy the 18-electron rule. Recently, Sawamura et al. [J. Am. Chem. Soc. vol. 124, pp. 9354 (2002)] have succeeded in synthesizing fused complexes of ferrocene and ruthenocene with fullerene, known as bucky-ferrocene and bucky-ruthenocene, respectively. The experiments show shift in charge density from ferrocene to fullerene in the ground state. However, no charge transfer from ruthenocene to fullerene is observed in case of the bucky-ruthenocene. We have performed all electron density functional calculations to obtain the equilibrium structures of the bucky-ferrocenes and bucky-ruthenocenes. Both, the staggered and eclipsed geometries are examined. The differences in the electronic structure and nature of bonding in these two systems are studied by analyzing the frontier orbitals, dipole moments, and charge density in their ground and singlet excited states.

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