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Structural and electronic properties of a bucky-ferrocene molecule from first-principles[1] JINWOO JEONG, YOUNG-GUI YOON, Chung-Ang University — Bucky-ferrocene molecules have been synthesized from fullerene and ferrocene molecules. The molecules have features of both components. We performed first-principles electronic structure calculations of a bucky-ferrocene based on C_{60} fullerene and ferrocene molecules in a supercell geometry. We got local minimum structures with geometry optimization from different initial configurations. Orientation of methyl groups and pentacene leads to states in small energy range. Possible device applications of the molecule are discussed.

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