第一原理計算による$(EDO\text{-}TTF)_2PF_6$の構造と電子状態に対する理論研究

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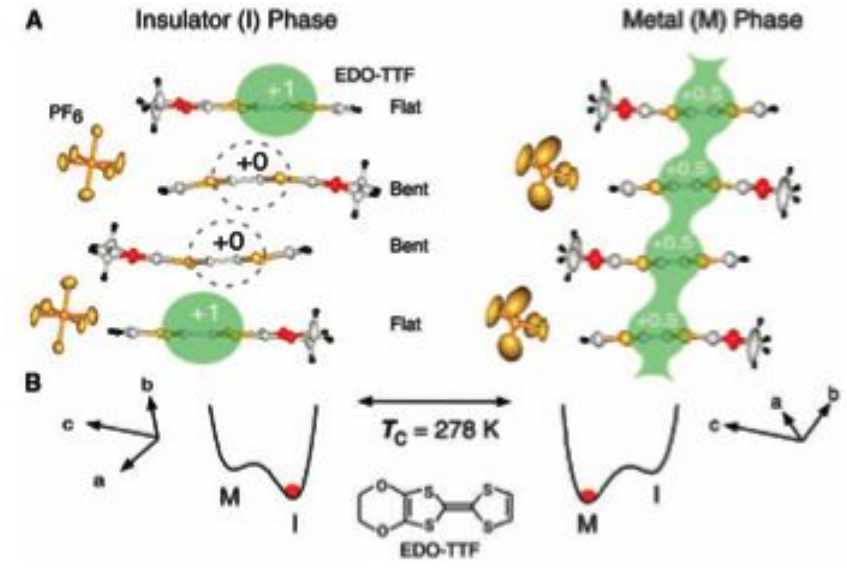

Fig. 1. (A) Schematic views of the lattice and electronic structural changes accompanying the M-I phase transition in $(EDO\text{-}TTF)_2PF_6$. A side view of an EDO-TTF molecule is shown. The unit cell includes two and four EDO-TTF molecules in M and I phases, respectively (*15*). In the I phase, holes are localized on EDO-TTF molecules with a flat structure due to CO, and quasi-neutral molecules show a bent structure. In the M phase, charges (holes) are delocalized and PF_6 (acceptor) molecules exhibit disorder (*15–18*). (**B**) Schematics for free-energy change accompanying M-I transition and the structure of the EDO-TTF molecule.

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二つの競合する相

絶縁相
- ２種類の分子構造
- 大きな分子変形
- 電荷秩序（[0110]type）
- anionの回転の自由度

LDAやGGAの精度は？