Simulation of organic conductors: TTF–TCNQ and $(TMTSF)_2X$

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Two types of one-dimensional organic conductors: TTF-TCNQ and $(TMTSF)_2X$ have been studied by density functional calculation. Our calculation is carried out using the projector-augmented wave method and a plane wave basis set. TTF-TCNQ is the first organic conductor to present a large conductivity in a wide temperature domain down to 59K, where a sharp metal to insulator transition is observed. $(TMTSF)_2X$ is a superconductive material.[1] We investigated the energetic information such as band structure and density of states. We also studied the impurity X in $(TMTSF)_2X$. The results could help us to learn the conductivity of the organic conductors better.

1. Denis Je´rome, Chem. Rev. 104 5565-5591 (2004)

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