Design of the tellurium-containing semiconducting polymers

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A series of donor-acceptor-donor (D-A-D) type semiconducting polymers containing tellurium atom in their acceptor units were designed and their structural and electronic properties were investigated by using density functional theory (DFT). Energy levels for highest occupied molecular orbitals and lowest unoccupied molecular orbitals were calculated, and then the electronic band gap values, which directly affects the electronic properties of the semiconducting polymers, were obtained for all the systems being investigated. The results of our investigations implied that the use of tellurium atoms in the acceptor units significantly decreases the electronic band gap which results with providing superior conducting properties to these polymers. Due to their superior electronic properties, these polymers may find important applications, such as in photovoltaic and electrochromic devices. During the study, we performed all DFT calculations by using Becke three-parameter hybrid exchange-correlation functional combined with Lee-Yang-Parr correlation functional and the LANL2DZ basis set.

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