Effect of Externally Introduced Carriers on the Electronic Structure of Fullerite and Fullerides

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We study the electronic structure of the pristine C60 fullerite with externally introduced carriers. From the density-functional study it is found that introducing electrons into the semiconducting C60 widens both valence and conduction bands. On the other hand, introducing holes is found to narrow them considerably. We also study the effect of the carrier introduction into the semiconducting body-centered cubic Cs6C60 fulleride, which is found to show similar band-width change and to become a good candidate for the superconductor.