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专刊

Theoretical XANES spectra for C_{76} isomers

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摘要

Two isolated pentagon rule satisfying isomers of C_{76} are optimized. And 1(D_2 isomer is reconfirmed to be the relative more stable one. The X-ray absorption near-edge structure (XANES) spectra are theoretically characterized by the hybrid density functional theory (DFT) method in combination with the full core-hole potentials. Isomer identification of XANES spectra for C_{76} is found and XANES spectra dependence on local structure of fullerene is discussed.

关键词

fullerene C_{76}, isomer, calculated XANES spectra, local structure dependence

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