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Energetic and structural properties of fullerenes under irradiation processes

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On the basis of the atomic displacement energy (T_d) calculated using the Density Functional Theory with Tight Binding Approximation (DFTB), the cross sections of electron-induced atomic displacement were obtained as a function of the order of the fullerene. Three types of defects commonly induced by radiation (mono-vacancy, di-vacancy and Stone-Wales) were also analyzed, determining their formation energies and the structural changes they produce in the molecule. The results are consistent with the model for the transformation of polyhedral structures to spherical nano-onions under electron irradiation, proposed by Ugarte in 1995.

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