MD simulation for hydrogen capture by boron-doped fullerenes at low energy collisions

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Theoretical study of the hydrogen uptake capability of carbon fullerene cages C60 and their boron-doped heterofullerene equivalents C59B is presented in this work. The fullerenes are irradiated by hydrogen atoms in an impact energy range of 0.1e100 eV. In order to predict exohedral and endohedral hydrogen captures as well as the scattering probability of hydrogen for various cage types and sizes, quantum-classical molecular dynamics (QCMD) calculations are used with the self-consistent-charge density-functional tight-binding (SCC-DFTB) method. Maximum endohedral hydrogen capture probabilities of 20% is found at impact energies close to 15 eV for both systems.
Similar results for the hydrogen capture are obtained by classical molecular dynamics based on the ReaxFF potential. Finally, the stopping cross section per carbon atom from the QCMD simulations for all cage sizes displays a linear dependence on the projectile velocity with a threshold at 0.8 eV, and extrapolates well to the available theoretical data.