Reaction barriers and deformation energies of C_{60}-based composites

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The current paper is aimed at the determination of barriers that govern the covalent coupling between two fullerenes C_{60} (C_{60} dimer), C_{60} and single-walled carbon nanotube ([C_{60}-(4,4)] carbon nanobud), and C_{60} and graphene ([C_{60}-(5,5)] and [C_{60}-(9,8)] graphene nanobuds). *Brutto* barriers determined as couplings energies E_{cpl}^{tot} are expanded over two contributions that present total energy of deformation of the composites' components E_{def}^{tot} and energy of covalent coupling E_{cov}^{tot}. In view of these energetic parameters and in contrast to expectations, seemingly identical reactions result in different final products. The peculiarity is suggested to be provided by a topochemical character of the covalent coupling between any two members of the sp^2 nanocarbons' family. The computations were performed by using the AM1 semiempirical version of unrestricted broken symmetry Hartree-Fock approach.