Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Graphene mechanics: I. Efficient first principles based Morse potential

Supplementary Material

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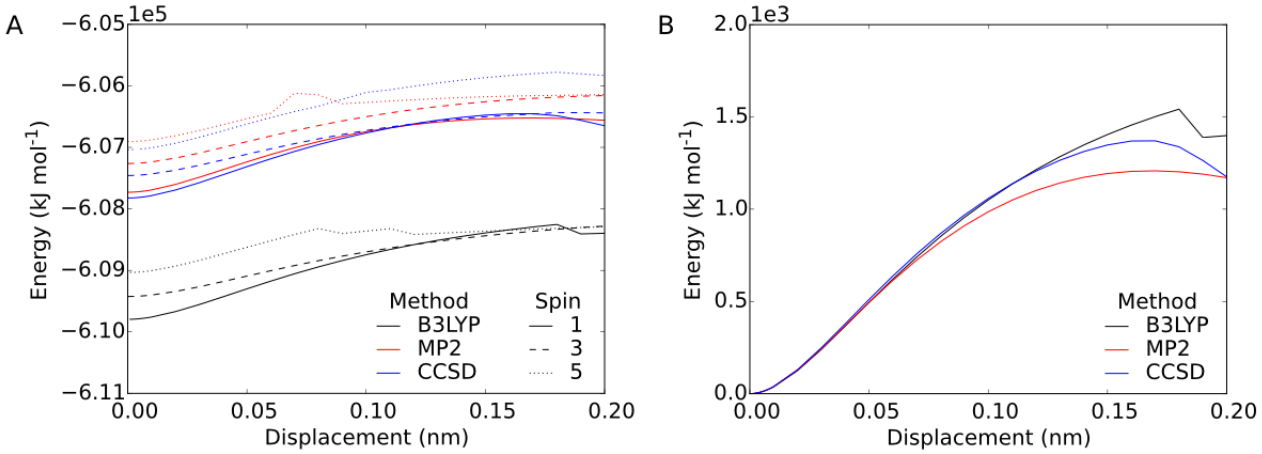

Fig. S1 Energy profiles of benzene dissociation as a function of distance between the fragments, calculated with several QM methods. The dissociation generates 2 mirror fragments, each with 3 C and 3 H atoms, and breaks two C-C bonds. Energy profiles are shown up to a distance of 0.2 nm, which is larger than the distance (0.12 nm) used in the fitting procedure (Fig. 4 of main article). We conclude that using B3LYP and the lowest spin multiplicity is appropriate for aromatic bond breaking. A) Absolute energy profiles show that the the singlet state is the most energetically favorable, independent of the method. B) The slope of the normalized energy profiles up to the inflection point is highly similar for the singlet state, independent of the method.