Evaluations of Interaction Energies for Larger Complexes and Endohedrals

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Relatively large molecular complexes can be at present observed and their various characteristics extracted from the experiments. This development calls also for related computations. Density functional theory represents a reasonable choice though it is still not clear which approximations should be most reliable for the purpose. For example, the Perdew and Wang PW91 functional has been suggested. The computations are carried out for several larger complexes including some fullerene endohedrals with a supposed weak interaction between the fullerene cage and encapsulate.