Fullerene Dimers and their Anions

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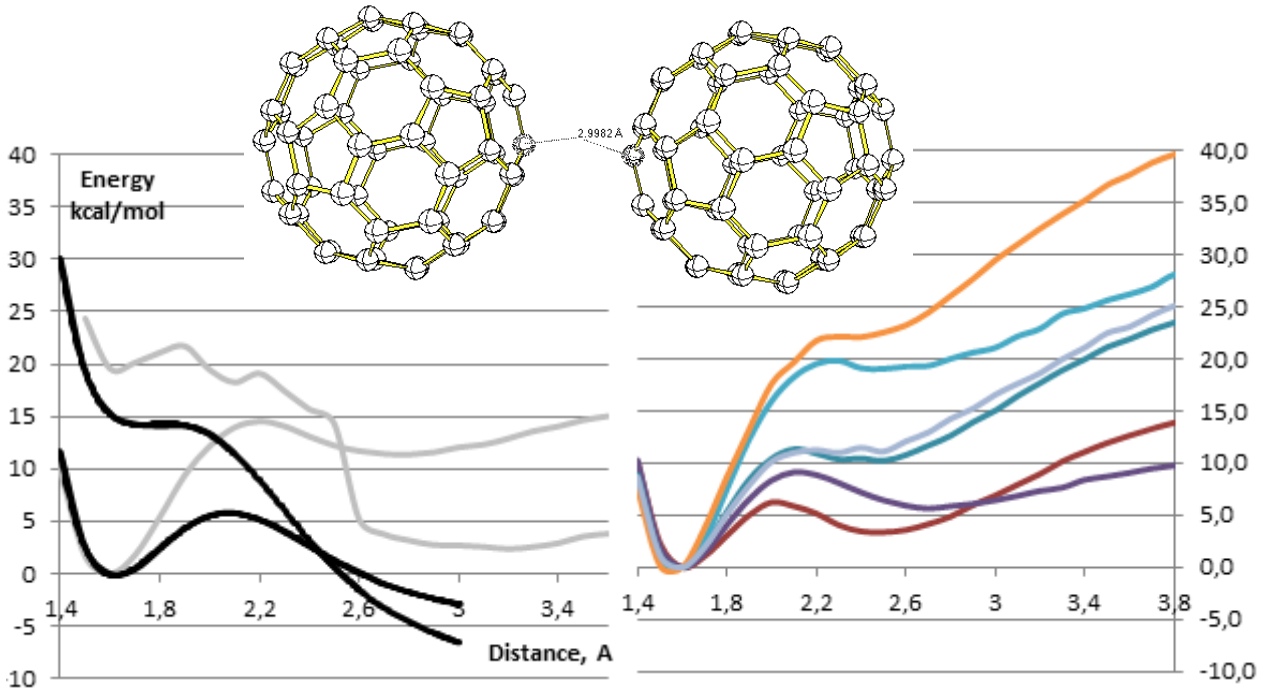

The interaction between two fullerenes is important for understanding the principles of electron transfer in fullerene-containing devices. Up to now, only two types of fullerene dimers were considered: the double-bonded neutral dimer [1] and the single-bonded dianion dimer [2].

We observed that there is one more minimum on potential energy surface of the system containing two fullerenes. This minimum corresponded to a Van-der-Waals bonded (non-bonded) dimer with distance between the surfaces of the fullerenes of 0.27-0.28 nm (≈ 1 nm between centers of buckyballs). That is the normal distance between fullerenes in crystal fullerite. The results of the calculations strongly depend on Hartree-Fock exchange and dispersion correction. Also for the dianion dimer crossing of spin-states between single-bonded and non-bonded dimer was observed. The stability of the ground state of the single-bonded dimer is comparable to that of the excited state of the van-der-Waals dimer.

Investigations of new dimer, spin-states crossing and electron transfer are in process.

DFT-calculations (PPE-scans) were performed using Becke 88 functionals with different HF exchange, BHHLYP and CAM-B3LYP functionals in ADF, NWChem and Gaussian.

[1] K. Komatsu, et al., *J. Org. Chem.*, **1998**, *63*, 9358-9366
[2] D. V. Konarev, et al., *Russian Chem. Bull, Int. Ed.*, **2011,** *60(6),* 1063-1070,