Absorption spectra of alkali-C_{60} nanoclusters

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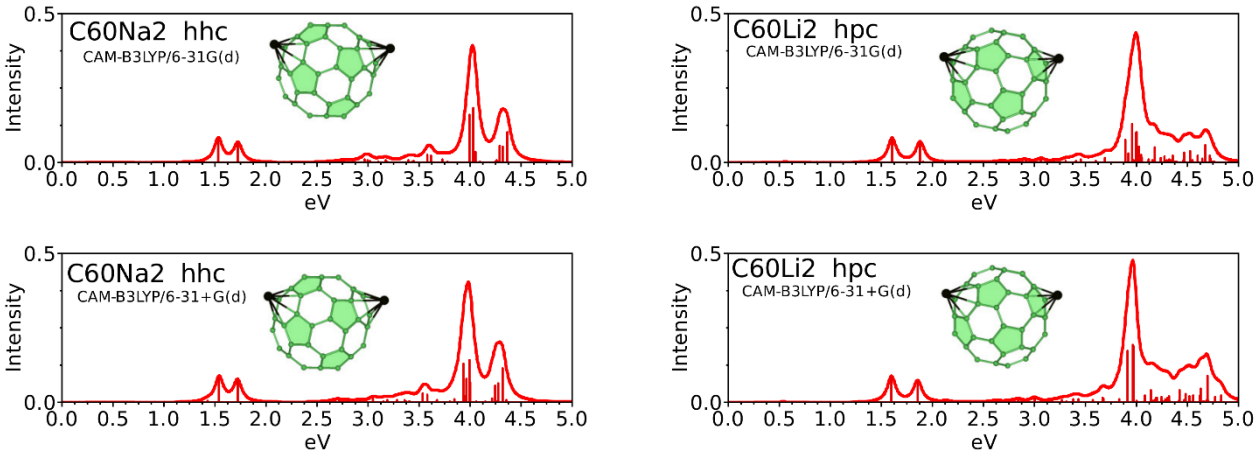
Supplementary information

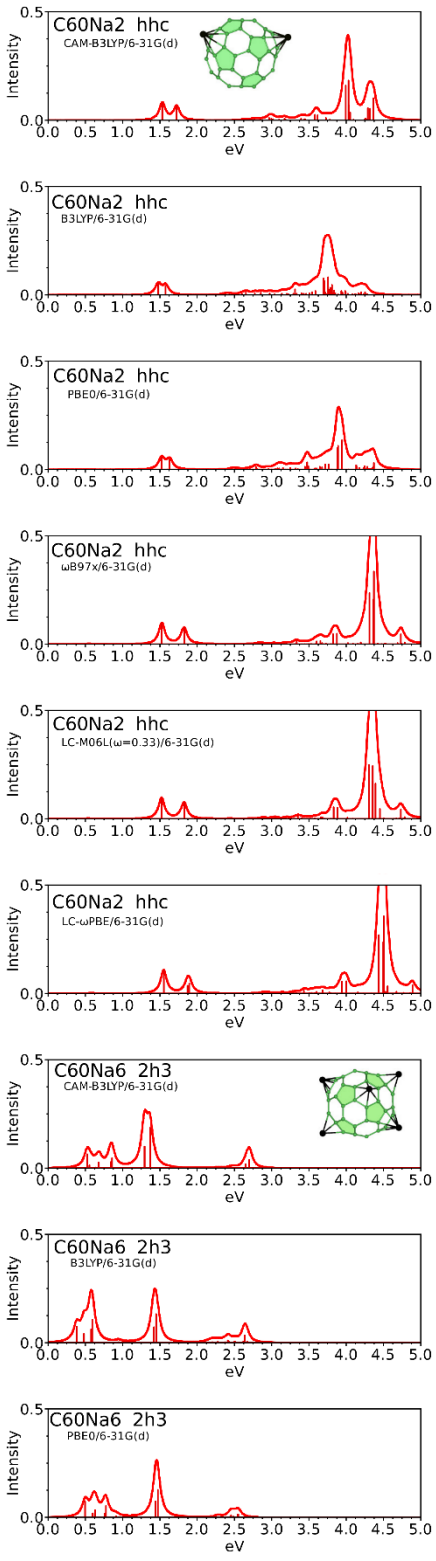
Figure S-1.



Absorption spectra of $C_{60}Li_2$ and $C_{60}Na_2$ calculated with CAM-B3LYP and using two Gaussian basis sets, namely 6-31G(d) and 6-31+G(d) [1]. Spectra are found to be very similar.

[1] J.D. Dill and J.A. Pople, *J. Chem. Phys.*, 1975, **62**, 2921; M.M. Francl, W.J. Petro, W.J. Hehre, J.S. Binkley, M.S. Gordon, D.J. DeFrees and J.A. Pople, *J. Chem. Phys*., 1982, **77**, 3654; V. Rassolov, J.A. Pople, M. Ratner and T.L. Windus, *J. Chem. Phys*., 1998, **109**, 1223.

Figure S-2.



Spectra of $C_{60}Na_2$ and $C_{60}Na_6$ calculated with several exchange and correlation functionals:

the hybrid B3LYP [2] and PBE0 [3], and the long-range-corrected ones ωB97x [4], LC-M06L(ω=0.33) [5], LC-ωPBE(ω=0.40) [6], and CAM-B3LYP [7].

Spectra are somewhat similar. In comparison with spectra calculated at CAM-B3LYP level, the main band obtained at B3LYP and PBE0 levels is slightly redshifted, while it is blueshifted by 0.3-0.4 eV at ωB97x, LC-M06L, LC-ωPBE levels.

[2] A. D. Becke, *J. Chem. Phys.,* 1993, **98**, 5648; C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785.

[3] C. Adamo, V. Barone, *J. Chem. Phys*, 1999, **110**, 6158-69.

[4] J. D. Chai, M. Head-Gordon, *J. Chem. Phys.*, 2008, **128**, 084106.

[5] H. Iikura, T. Tsuneda, T. Yanai, K. Hirao, *J. Chem. Phys.*, 2001, **115**, 3540-3544; Y. Zhao, D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101.

[6] O. A. Vydrov, J. Heyd, A. V. Krukau, G. E. Scuseria, *J. Chem. Phys.*, 2006, **125**, 074106.

[7] T. Yanai, D. P. Tew, N. C. Handy, *Chem. Phys. Lett*., 2004, **393**, 51-57.