A density functional study of carbon monoxide on pristine and Li-encapsulated fullerene-like BeO

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Abstract

We report adsorption energies, structures, energy gap (E_g), charge transfer and electronic properties of carbon monoxide (CO) on primary, Li-encapsulated fullerene-like beryllium oxide ($Be_{16}O_{16}$, $Li^+@Be_{16}O_{16}$, $Li@Be_{16}O_{16}$, respectively) for several adsorption states. The results have been interpreted by DFT calculations. The presented evidence is that shows that the CO molecule is not strongly adsorbed on the fullerene-like $Be_{16}O_{16}$ on, leading to energy release of -0.17 to -0.4 eV while its electronic properties is not significantly changed. $Li^+@Be_{16}O_{16}$, $Li@Be_{16}O_{16}$, can adsorb carbon monoxide more strongly than their pristine fullerene-like $Be_{16}O_{16}$. The energy gap (E_g) of the $Li@Be_{16}O_{16}$ is significantly decreased from 3.51 to 2.88 eV upon the CO adsorption corresponding to the most stable configurations, respectively. It was shown that the electrical conductance of the $Li@Be_{16}O_{16}$ may be increased after the CO adsorption. It was found that the electronic properties of $Li@Be_{16}O_{16}$ are sensitive to the presence of CO molecule.

References

[1] K. Joshi. R. Jain. R. Pandya. B. Ahuja, B. Sharma, J. Chem. Phys. 111 (1999) 163.
[2] L. Ren. L. Cheng. Y. Feng, X. Wang, The Journal of chemical phys 137 (2012) 014309.
[3] M. Zhou. Z. Yi. K. Li. J. Zhang, W. Wu, Nan.Res. lett. 6 (2011) 1.
[4] D.-Y. Hwang, A. M. Mebel, Chem. Phys lett. 348 (2001), 303.
[5] M. Noei. V. Zare-Shahabadi, S. N. Razi, Chin. J. Chem. Phys. 26 (2013) 612.
[6] R. Shinde, M. Tayade, J. Phys. Chem. C 118 (2014) 17200.

Figures

(a)Structure of optimized Li into $Be_{16}O_{16}$ fullerene-like (endohedral), (b) Models for stable adsorption of CO on the $Li@Be_{16}O_{16}$ fullerene-like, and their density of states (DOS) plot. Bonds are in Å