

An ab initio study of optical and Raman spectra of heavily Li-doped 4 Å carbon nanotubes

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2006 J. Phys.: Condens. Matter 18 10115

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Erratum

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Professor B K Agrawal 2006 *J. Phys.: Condens. Matter* **16** 1467–1488

Our corrected cohesive energy for the bulk Li is in fact 1.82 eV (in contrast to the value reported in the paper, 0.5 eV) against the experimental value of 1.63 eV. When the binding energies are now calculated after taking the bulk Li energy as the reference energy, the calculated binding energies turn out to be more or less in agreement with the values of Liu and Chan [1]. The authors apologise to Liu and Chen for the unfounded criticism of their work in the paper.

None of the results of the above paper depends upon the bulk Li energy and therefore our results for the binding energies presented in the various tables which have been obtained after taking the isolated Li atom energy as the reference energy remain unaffected. Thus all the results for the binding energies, electronic structure, optical absorption and Raman active radial breathing mode frequencies obtained are technically sound and free from error.

References

- [1] Liu H J and Chan C T 2003 *Solid State Commun.* **125** 77