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Curvature effect on Carbon nanotube energy : Ab-initio calculation by cluster design

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Ab initio total energy calculation of carbon nanotube (CNT) has shown that the energy of CNT is inversely proportional to its radius due to the strain energy. However, limited scale of the ab initio calculation restricted the investigations to the range of the CNT radius less than 10. In order to calculate the total energy of CNT of larger radius, we suggested a clustering approach where the binding energy between carbon atoms is extracted from a small cluster representing the whole CNT. The cluster is a small fragment of flat graphite of which edges are passivated by hydrogen. From the linear relationship between the total energy and the size of the cluster, the total energy of graphite could be obtained by extrapolation. In this method, the radius of CNT can be presented by the curvature of the curved cluster, without increasing the total size of the system. Therefore, it was possible to extend the calculation to the CNTs of very large radii. As the radius of CNT increased, the total energy of the CNT decreased as in the previous works. However, the energy of the CNT converged to that of flat graphite when the radius of the CNT was larger than 37. CNTs of radii larger than 10 nm that are frequently observed in experimental works can be thus treated as flat graphite in the view of total energy.