

Simulation of STM and STS images of defects in nanotubes

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We present a *ab-initio* Density Functional Theory simulation of scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) of a semiconducting carbon nanotube with a sharp bend. This bend corresponds to a 'buckle' formed by mechanical strain. We have calculated the effects of these structural distortion on the electronic properties. Our simulations showed the formation of localized states inside the semiconducting gap. This results are in good agreement with recently measured STM spectra. [1]

References

- [1] J.W. Janssen, S.G. Lemay, M. van den Hout, M. Mooij, L.P. Kouwenhoven, and C. Dekker, *Kirchberg 2001 Conference Proceedings*, edited by H. Kuzmany, J. Fink, M. Mehring, and S. Roth, AIP Conf. Proc. No. 591 (AIP, Melville, NY, 2001), pp. 293-297