Contribution ID: **10** Type: **Oral Presentation**

# Studies of thermodynamic, structural and electronic properties of substitutional defects in models of single-walled carbon and boron nitride nanotubes

*Wednesday, 13 July 2011 11:15 (15 minutes)*

<p>We report on studies of thermodynamic, structural and electronic properties of substitutional defects involving C, B, N and vacancies in models of single-walled carbon and boron nitride nanotubes. Using the generalized gradient approximation (GGA) for the exchange-correlation functional, we perform first principles calculations within the framework of density functional theory to optimize fully the geometries of the systems in their ground states. We give detailed accounts of the relaxed geometries. We compare the heats of formation of the various point defects, and we draw conclusions about the relative stability of the these defects. We study the changes to the electronic structure for these defect systems, and further investigate the detailed nature of the defects. We make a comparative study of the C and BN nanotube systems.Where data is available, comparisons are made.

## Level (Hons, MSc, <br>   PhD, other)?

PhD

## Consider for a student <br>   award (Yes / No)?

Yes

## Would you like to <br> submit a short paper <br> for the Conference <br> Proceedings (Yes / No)?

No

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**Session Classification:** CMPMS1

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