Contribution ID: **17** Type: **not specified**

Structural, electronic and optical properties of the two isomers of Si(111)2x1

Friday, 20 January 2012 17:00 (20 minutes)

The Si(111)2x1 surface, which appears on cleaved surfaces at low and room temperature, has been among the most studied semiconductor surfaces ever.
Although apparently simple, it shows several intriguing and not completely understood features.
The atomic structure of the Si(111)2x1 surface has been known for decades to consist of Pandey chains [1], that can tilt with two possible directions, generating two almost degenerate structures called isomers: the Si(111)2x1 negative buckling and the Si(111)2x1 positive buckling.
Although it is currently believed that for a sample of Si(111)2x1 at room temperature the most stable configuration is the positive buckling structure[2], it has been recently shown by STS measurements that for highly n-doped Si(111)2x1, at low temperature, both positive and negative isomers may coexist on the surface [3].
A confirmation of this experimental observations could come from the study of optical properties of these two isomers.
In this talk I will show and discuss the results of our theoretical simulations for the calculation of structural, electronic and optical properties (RAS spectra [4]) of the two structures, obtained by ab-initio calculations within the most reliable state-of-the-art methods based on density functional theory and many-body perturbative techniques.

References:

[1] K. C. Pandey, Phys. Rev. Lett. 47, 1913 (1981)
[2] S. Nie et al., J. Vac. Sci. Technol. A 22(4), 1671 (2004)
[3] G. Bussetti et al., Phys Rev. Lett. 106, 67601 (2011)
[4] for a Review see for example P. Weightman, et al., Rep. Prog. Phys. 68, 1251

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Session Classification: Session - IV : Astrophysics and Condensed Matter Applications