Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Reflectance Anisotropy Spectroscopy(RAS) of Si(111)-(3x1)-Ag and Si(111)-c(12x2): Comparison of hybrid density functional theory and experiment[1] SOFIA JORGJI, JOHN MCGILP, CHARLES PATTERSON, Trinity College Dublin, Ireland — The atomic and electronic structures of the Si(111)-(3x1)-Ag surface have been investigated extensively by LEED, STM and electron spectroscopies. The atomic structure is believed to be a honeycomb chain plus channel (HCC) structure in which channels containing Ag atoms are separated by Si in honeycomb chains. Here we compare results of previous reflectance anisotropy spectroscopy (RAS) experiments with hybrid DFT simulations for the HCC structure. Results of RAS simulations are in very good agreement with RAS experiments and indicate that the HCC structure is likely to be correct. Surface state features responsible for the RAS signal are identified and the effect of dimerisation of Ag chains on the RAS spectrum is considered.

[1]This work was supported by the Irish HEA under PRTLI-V

Sofia Jorgji
Trinity College Dublin

Date submitted: 08 Nov 2012 Electronic form version 1.4