Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Potassium-induced semiconducting to metallic transition on the β-SiC(100) c(4x2) surface BARRY HAYCOCK, Dublin Institute of Technology / West Virginia University — We present new data on the potassium-induced semiconducting to metallic transition of the silicon-terminated β-SiC(100) c(4x2) surface, resulting from density functional theory simulations. In our calculations we have analysed many different K-SiC(100) structures, corresponding to K coverages ranging from 0.08 to 1.25 monolayers (ML), paying special attention to the 2/3 ML and 1 ML cases where the transition has been reported. We find that the K-SiC(100) surface is metallic in all the cases. In spite of that, the K layer shows a semiconducting density of states (DOS) up to K coverages of $\sim$1ML, beyond which the potassium layer undergoes a transition to metallic behaviour, explaining the experimental observation. We propose a new atomic model for the surface reconstruction of the 1ML case which has far lower total energy than the previously suggested model based on linear K chains after simulated annealing studies.

Barry Haycock
Dublin Institute of Technology / West Virginia University

Date submitted: 27 Nov 2010 Electronic form version 1.4