Abstract Submitted
for the CAL09 Meeting of
The American Physical Society

Computational study of the adsorption of methanol, formic acid, and formaldehyde on the β-SiC(100)-3x2 surface LEKH ADHIKARI, SEAN CASEY, University of Nevada, Reno — The absorption of methanol, formic acid, and formaldehyde on the Si-rich β-SiC(100)-(3x2) surface has been studied using density functional theory (DFT) computational methods and small clusters to model the surface reactivity. A single cluster dimer model is used to calculate energies after the interaction of adsorbates on the surface. The dissociative adsorption of methanol on the SiC(100)-3x2 surface is predicted to take place facilely, giving rise to Si-OCH_3 and Si-H surface species and followed a path similar to that predicted for Si(100)-2x1 surface. The reaction is highly exothermic and predicted to occur with essentially no barrier. Formaldehyde is also predicted to adsorb with essentially no barrier on the SiC(100)-3x2 surface with formation of a 4-member ring on the surface. This adsorption is also exothermic and similar to the corresponding Si(100)-2x1 surface. This result shows that the carbonyl group can undergo cycloaddition onto the SiC(100) surface. Formic acid is also predicted to undergo dissociative chemisorption on the SiC(100) surface with the formation of Si-OCOH and Si-H surface species. This process is also highly exothermic (-283.1 kJ/mol) and essentially barrierless.

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Date submitted: 05 Oct 2009 Electronic form version 1.4