Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

The Structure of Adsorbed Methane on the MgO(100) Surface from Inelastic Neutron Scattering and First-Principles Calculations M.L. DRUMMOND, B.G. SUMPTER, W.A. SHELTON, JR., Oak Ridge National Laboratory, J.Z. LARESE, University of Tennessee — The adsorption of molecules onto a solid surface is a phenomenon with important ramifications in areas such as catalysis, corrosion, and electronics. We have used plane-wave, psuedopotential-based density functional calculations, in conjunction with inelastic neutron scattering (INS), to evaluate the structure of methane on the MgO(100) surface. The combination of high-resolution INS and high-quality calculations has proven extremely versatile in determining the structural arrangement, despite the existence of multiple energetically favorable arrangements. The structures for adsorbed methane mono-, bi-, and higher order adlayers are discussed.

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Date submitted: 11 Jan 2006 Electronic form version 1.4