Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Simulation of methane on Al(111)[1] MAJID KARIMI, CARL LEBLOND, IUP, WAHYU SETYAWAN, STEFANO CURTAROLO, Duke University, RENEE DIEHL, Penn State University, DUKE UNIVERSITY COLLABORATION, PENN STATE UNIVERSITY COLLABORATION, IUP COLLABORATION — Classical many-body interatomic potentials for methane molecules interacting with Al(111) are developed using the embedded-atom method (EAM). The optimized EAM parameters for methane-Al(111) are obtained by fitting to the data generated from the first principles calculations. Adsorption of methane on the Al(111) substrate is studied using the Grand Canonical Monte-Carlo method. Adsorption isotherms are calculated at several temperatures near the triple point temperature of methane Tt = 90K, and structural parameters obtained from the adsorbed density profiles. The structures and the thermodynamics of film growth are compared to methane adsorption on other metal surfaces, graphite and the d-Al-Co-Ni quasicrystal. This research is supported by NSF and ACS-PRF.

[1]This research is supported by NSF and ACS-PRF

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Date submitted: 19 Nov 2008 Electronic form version 1.4