Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Simulations of adsorption of hydrocarbons on decagonal Al-NiCo quasicrystal surfaces WAHYU SETYAWAN, Duke University, RENEE D. DIEHL, MILTON W. COLE, Pennsylvania State University, STEFANO CURTAROLO, Duke University — Classical many-body interatomic potentials for hydrocarbon adsorptions on Al-Ni-Co systems are developed by using the Embedded-Atom Method. The potentials are fit to ab-initio energies of Al-Ni-Co ternary phases and hydrocarbons adsorbed on decagonal surface of Al-Ni-Co (d-AlNiCo) approximants. First principle data show that no dissociation occurs for all systems in the training set, indicating no chemisorptions. We extend the study and use the potentials to simulate adsorption of simple hydrocarbons on d-$Al_{73}Ni_{10}Co_{13}$ quasicrystal surfaces using Grand Canonical Monte Carlo method. Research sponsored by ACS and NSF.

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Date submitted: 26 Nov 2007 Electronic form version 1.4