Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Multisite Interactions in Lattice-Gas Models of Adsorbates: Reconciling Adatom Relaxations at Steps[1] T.L. EINSTEIN, RAJESH SATHIYANARAYANAN, T.J. STASEVICH[2], U. of Maryland — In a lattice-gas (LG) framework for (111) cubic surfaces, pair interactions cannot distinguish A and B steps, but an orientation-dependent three adatom (trio) interaction can, as we verify with VASP for Cu(111).[3b] However, on Pt(111), small clusters considerably underestimate the difference.[4] For a sequence of overlayer configurations, we explore the role of lateral relaxations and how they complicate LG analysis. On Cu(100) our prior VASP calculations of a particular trio interaction energy (E_d) gave a large positive value.[3c] This nearly cancels the attractive second-neighbor interaction energy (E_2), leading to a discrepancy between theory and experiment of step stiffness anisotropy.[3a] Relaxations at step edges greatly reduce this repulsion. Since position-dependent interactions are improper in LG models, we show how to deal with this phenomenon using a quarto interactions. We comment on extensions to (110) faces and analytic expressions for step stiffness.

[1]Supported by NSF MRSEC Grant DMR 05-20471, partially by DOE CMSN DEFG0205ER46227. Computing done at NCSA (NSF), UIUC.
[2]Now at Lab Receptor Biology, Nat'l Cancer Inst., NIH, Bethesda
[3]TJS et al., PRB a)**70**('04)245404, b)**71**('05)245414, c)**73**('06)115426.
[4]Feibelman, Surf. Sci. **463**('00)L661; Michely et al., ibid. **256**('91)217.

Theodore Einstein
University of Maryland, College Park

Date submitted: 20 Nov 2006 Electronic form version 1.4