

Abstract Submitted  
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**Ab-initio Evaluation of Extended Lattice Gas Interactions of Cu on Cu(111) and Cu(001)**<sup>1</sup> T. J. STASEVICH, T. L. EINSTEIN, University of Maryland, College Park, S. STOLBOV, Kansas State University — Lattice gas models connect macroscopic evolution to microscopic energies. The traditional empirical parameterization of these models can lead to incomplete descriptions that yield effective rather than actual energies. More recently, self-consistent computations from first principles of the relevant interaction energies can be used to diminish the risk of incompleteness. We have used such an approach to calculate a variety of lattice-gas interaction energies between Cu adatoms on Cu(001) and Cu(111). We find that pair interactions beyond first neighbors are negligible on Cu(111), whereas second neighbor interactions are significant on Cu(001). Besides pair-interactions, we find that trio-interactions can also be quite large. On Cu(111) these include two orientation dependent trios that account for the difference in the formation energies of A- and B-steps. When taken together, the calculated interaction energies are self-consistent and compare well with previous theory and experiment <sup>2</sup>.

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<sup>2</sup>T. J. Stasevich et al., Phys. Rev. B 70, 245404 (2004); 71, 245414 (2005)

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