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Role of Adatom Relaxations in Computing Lattice-gas Energies: Multisite Interactions[1] RAJESH SATHIYANARAYANAN, T. L. EINSTEIN, Univ. Maryland, College Park — In simple lattice-gas models, only nearest-neighbor pair interactions are used to model adatom interactions. However, multisite interactions, such as trios and quartos, are necessary to understand certain surface properties like the orientation dependence of step stiffness and the equilibrium shape of islands. Strong multisite interactions are found to be present on a variety of metallic surfaces. Unlike pair interactions, the relaxations of adatoms in a multisite interaction are not along bond directions. Hence, these adatoms can shift significantly from their high-symmetry positions, making multisite interactions more sensitive to relaxations. Using VASP calculations, we showed that trios are very sensitive to lateral adatom relaxations on Pt(111) and Cu(100)[2]. Our recent calculations on Cu(110) indicate that in addition to trios, quartos also undergo a big change due to adatom relaxations. Such findings severely limit the effectiveness of lattice-gas models in characterizing surface interactions. We discuss alternate approaches to this problem.

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[2]Rajesh Sathiyanarayanan *et al.*, Surf. Sci. **602** (2008) 1243.

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