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Connector Model for Many-Body Interactions at Surfaces from First Principles[1] YOGESH TIWARY, KRISTEN FICHTHORN, The Pennsylvania State University — First-principles calculations based on DFT indicate that pair, trio, four- and five-body atomic interactions are significant in Al clusters on Al(110). These many-body interactions are a signature of "elastic screening" of long-ranged, substrate-mediated, elastic interactions between atoms in dilute adlayers by direct bonding and short-ranged substrate relaxation in dense clusters. As a consequence of this screening, we developed the Connector Model to effectively describe the energies of compact clusters. Adsorbate structures and interactions are described in terms of single-atom, many-body connector units, which link to one another to form the structures that can occur in thin-film and crystal growth. The additive connector energies can be effectively incorporated into a lattice-based Hamiltonian to study thermodynamics and kinetics at surfaces. The Connector Model is considerably more efficient than lattice-gas Hamiltonian approaches, which would require a large number of terms to accurately capture many-body effects. Details of the connector model and its application to predicting the shapes of compact clusters on Al(110) including the chain-to-island transition will be discussed. This model can be extended to other crystalline surfaces.

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Yogesh Tiwary
The Pennsylvania State University

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