Abstract Submitted
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**Surface Step Stiffness: Next-Nearest Neighbor Interactions and Beyond**[1] T. J. STASEVICH, T. L. EINSTEIN, U. of Maryland, College Park — Most theoretical treatments of the orientation-dependence of step stiffness consider only attractive nearest-neighbor (NN) interactions. Recent experiments[2] on Cu(100) suggest that this approximation leads to an underestimation of the measured stiffness for orientations far from close-packed directions. Including attractive next-nearest-neighbor (NNN)[3] and/or right-triangle trio interactions (consisting of two NN legs and one NNN hypotenuse) can ameliorate the discrepancy.[4] Reaching good agreement, however, may require other, more novel interactions. To determine which of these are most relevant, we have performed ab-initio calculations using VASP, seeking the relative strengths of NN, NNN, and various trio interactions on Cu(100) and Cu(111) surfaces. On Cu(100) we find that NNN interactions are indeed attractive and relatively large (consistent with experimental results). We also find a significant attractive right-triangle trio interaction, as well as a repulsive linear trio interaction. On Cu(111), in contrast, we find that NNN interactions are negligibly small, again consistent with experiment [5]

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