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Ab initio calculation of atomic interactions on Al(110): implications for epitaxial growth[1] KRISTEN FICHTHORN, YOGESH TIWARY, Penn State University — Using first-principles calculations based on density-functional theory, we resolved atomic interactions between adsorbed Al atoms on Al(110). Relevant pair and trio interactions were quantified. We find that pair interactions extend to the third in-channel and second cross-channel neighbor on the anisotropic (110) surface. Beyond these distances, pair interactions are negligible. The nearest-neighbor interaction in the in-channel direction is attractive, but nearest-neighbor cross-channel interaction is repulsive. While nearest-neighbor, cross-channel repulsion does not support the experimental observation of 3D hut formation in Al/Al(110) homoepitaxial growth [1], we find that trio interactions can be significant and attractive and they support cross-channel bonding. The pair and trio interactions have direct and indirect components. We have quantified the electronic and elastic components of the indirect, substrate-mediated interactions. We also probe the influence of these interactions on the energy barriers for adatom hopping. [1] F. Buatier de Mongeot, W. Zhu, A. Molle, R. Buzio, C. Boragno, U. Valbusa, E. Wang, and Z. Zhang, Phys. Rev. Lett. 91, 016102 (2003).

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