

Abstract Submitted
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An Electronic View of the Step-edge Schwoebel Barrier Problems YINA MO, Harvard University, ZHENYU ZHANG, Oak Ridge National Lab, University of Tennessee, EFTHIMIOS KAXIRAS, Harvard University — Using First-principle calculations, we studied the energetics of adatoms Co, Fe, Cu, and Zn on the stepped Cu(111) surfaces and that of adatoms Rh, Pd, and Ag on the stepped Pd(111) surfaces. We found that the behavior of the adatoms at the step edge of these substrates is governed by the electronic interactions instead of strain effects. The different energetics and kinetics of the different adatoms on the same substrates result from the difference in which these adatoms *see* the charge distributions from the identical substrates. We further clarified that atomic level studies of these cases are required because the bond counting rules are not universal.

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