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Electronic origin of kinetic and dynamic processes at atomic steps on vicinal metal substrates¹

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Single-atomic-layer steps play an important role in the kinetics and dynamics of morphological evolution and structural formation at surfaces. In this talk, we will attempt to elucidate the importance of the electronic nature in determining the bonding of adatoms and the activation barriers for adatom descent at step edges. The insights gained through first-principles case studies have timely and important impacts in understanding the evolution of many nanostructured surfaces and prevention of electrical breakdown in nanodevices. In the first case [1], we establish a clear correlation between the preferred diffusion mechanism and step-edge barrier and the relative degree of electronic shell filling of the adatom and the substrate. We also find an approximate linear relation between the adatom step-edge hopping barrier and the adatom-surface bonding strength with a slope roughly proportional to the number of the nearest neighbors of the adatom in the initial state. These results can serve as simple guiding rules for predicting precise atomic surface morphologies and designing desirable surface nanostructures, such as atom wires [2]. In the second case [3], we discover an optimal surface electromigration inhibitor on the technologically important Cu(111) surface, characterized by energetically favoring and binding strongly at the kink of step edges. Finally, we will briefly discuss how the electronic bonding strengths influence the nucleation and growth behavior of carbon atoms at the step edges of various transition-metal surfaces, a crucial insight in designing optimal kinetic pathways for mass production of quality epitaxial graphene [4].

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