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Insights in to hetero diffusion and growth: A DFT Study H. YILDIRIM, SUBRAMANIAN SANKARANARAYANAN, JEFF GREELEY, Argonne National Laboratory — We report the results of first principles calculations performed to study heteroatom diffusion on the terraces and step edges of fcc(001) surfaces on a series of 3d, 4d and 5d transition metals. For each adsorbate-substrate pair, we report the most stable adsorption sites and the corresponding adsorption energies. The corresponding terrace diffusion barriers are also reported, and periodic trends in the barrier heights are related to differences in adsorbate adsorption energies, cohesive energies of both adsorbate and substrate, and the differences in bond length/strength. Diffusion barriers and mechanisms at the step edges are also reported. Finally, insights into the possibility of 2D vs. 3D growth for each studied system are discussed via the calculated Ehrlich-Schwoebel barriers.

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