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Modeling Adsorption on fcc(nnm) Surfaces[1] ALAIN PHARES, Villanova University, DAVID GRUMBINE, JR., St. Vincent College, FRANCIS WUNDERLICH, Villanova University — In general, fcc(nnm) surfaces consist of very long armchair (111) terraces separated by steps. The number M of atomic sites in the width of the terraces depends on the Miller indices (nnm). The model considers values of $M \leq 6$, with adsorbate-substrate interaction energy on step-sites different from those on bulk sites, takes into account first- and second-neighbor adsorbate-adsorbate interactions, and specializes to the case of attractive first-neighbors. We obtain the complete low temperature, 3-dimensional, energy phase diagrams. The occupational configurations of the phases exhibit features similar to those of the phases obtained in the infinite-width limit, or flat fcc(111) surfaces. This yields a classification of the phases into types, and, within each type, the phases are grouped into families. This suggests a number of generalizations for any value of M beyond 6, leading to a better understanding of the competing interaction energies and of the evolution of the phase diagrams with increasing width M of the terraces. The relevance of these results to experiments is discussed within the context of preferential adsorption on step sites, and applied to the adsorption of water on Pt(335).

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