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Adsorbate-Induced Faceting of Ir and Re Surfaces PAYAM KAGHAZCHI, TIMO JACOB, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, 14195 Berlin, Germany, WENHUA CHEN, HAO WANG, THEODORE MADEY, Rutgers University, NJ 08854, USA — Since high-index clean metal surfaces typically have lower surface atom densities and higher surface free energies compared to the close-packed surfaces of the same metal they can be used as the basis for surface reconstruction and facet formation studies. In this context experimentally we found recently that on Ir(210) and Re(11$\bar{2}$1) surfaces strongly interacting adsorbates are able to induce the formation of well defined nanostructures after annealing the system at elevated temperatures. Using density functional theory calculations with the PBE functional and *ab initio* atomistic thermodynamics we studied the adsorption of oxygen and nitrogen on the different surface orientations, which are involved in the nanostructures on Ir(210) and Re(11$\bar{2}$1). Constructing the corresponding (p, T)-surface phase diagrams, we find that at experimental pressure conditions ($p_{O_2} = 5 \cdot 10^{-10}$ atm) above 1100 K for Ir and above 1200 K for Re the planar surfaces are stable, while lowering the temperature stabilizes the nanofacets found experimentally. While on Ir(210) most nanoscale pyramids consist of smooth and unreconstructed planes, some (110) faces show a stepped double-missing row superstructure, which is only stable on the faceted surface and at higher temperatures.

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