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Nature of Versatile Chemisorption on TiC(111) and TiN(111)¹

BENGT I LUNDQVIST, CARLO RUBERTO, ALEKSANDRA VOJVODIC, Department of Applied Physics, Chalmers University of Technology, SE-412 96, Göteborg, Sweden — Extensive density-functional calculations on the polar TiX(111) (X = C, N) surfaces show (i) for the clean surfaces strong Ti3d-derived surface resonances (SR's) at the Fermi level, unlike on the stable TiX(001) surfaces, and X2p-derived SR's in the upper valence band, and (ii) for chemisorption of atoms in the first three periods pyramid-shaped trends in atomic adsorption energies Eads, with an extremely strong O-atom bond. The adsorption is successfully described by a by us proposed concerted-coupling model (CCM), where adsorbate states couple to both kinds of SR's in a concerted way, and which is consistent with trends in the adsorbate-induced DOS and explains the characteristic variations in Eads and in bond lengths, as well as radical differences between TiX(111) and TiX(001), and similarities and small differences between TiC and TiN. The versatility of chemisorption on TiX(111) and the general nature of CCM indicate both ramifications and predictive abilities in, e.g., growth and catalysis.

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