The surface energy and band structure of γ-WO3 thin films

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**Ключевые слова:** WO3, thin film, surface energy, band structure **Abstract/Аннотация:** By means of ab initio calculations we demonstrate sizable anisotropy in surface energy of the γ-WO3 (001), (010) and (100) surfaces. The (001) surface has the smallest surface energy followed by the (010) and (100) surfaces. Their surface band structures are characterized by dispersion of bands near the gap region and by band-gap values similar to the ones of the bulk. The role of surface atoms in stabilizing the band gap is revealed. Variations in the position of the Fermi level are traced with respect to the different surface reconstructions.

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