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Driving force for the WO3 (001) surface relaxation MACIEJ GUTOWSKI, Pacific Northwest National Laboratory, IVAN YAKOVKIN, Institute of Physics of National Academy of Sciences of Ukraine — The optimized structure of the (001) WO_3 surface with various types of termination has been studied at the density functional theory level with a Perdew-Wang exchange-correlation functional. In contrast to transformations of bulk WO3, surface relaxation results in a significant decrease of the total energy. Indeed, the surface energy decreases from $10.2\text{x}10^{-2}$ eV/A^2 for the ideal (ReO_3-like) to $2.2\text{x}10^{-2}$ eV/A^2 for the relaxed c(2x2) O-terminated surface. The surface relaxation is accompanied by a dramatic redistribution of the density of states near the Fermi level, associated with transformations of surface states. This redistribution lowers the electronic energy of the slab and therefore is suggested to be the driving force for surface relaxation of the (001)WO_3.

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