

Abstract Submitted
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First-principles investigation of the structural, mechanical and electronic properties of the NbO-structured 3d, 4d and 5d transition metal nitrides¹ ZHI LIU, University of Toledo, XIUQUAN ZHOU, University of Maryland, DANIEL GALL, Rensselaer Polytechnic Institute, SANJAY KHARE, University of Toledo — We performed ab initio calculations on 29 transition metal nitrides from the 3d, 4d and 5d rows, in NbO structure. We calculated cohesive energy, lattice constant and elastic constants C_{11} , C_{12} and C_{44} , and derived mechanical moduli, related ratios and hardness. For five of the ten 3d transition metal nitrides, cohesive energy in this new structure is similar to that of the same composition in the rocksalt structure. The lattice constant and bulk modulus were found to be anti-correlated. We observed the correlation between the shear modulus (G), Pugh's ratio (k) and derived Vickers hardness (H_V). The nitrides, CrN, MoN and WN in NbO structure show values of H_V larger than 20 GPa. We showed systematically that C_{44} , G , k and H_V are anti-correlated with the number of electronic states around E_F . The local density of states demonstrating systematic evolution of the electronic structure was studied. Bader charge transfer analysis was performed. This work has been published as Liu et al., *Comput. Mater. Sci.* 84, 365 (2014).

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