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Super Hard Cubic Phases of Period VI Transition Metal Nitrides: A First Principles Investigation[1] S.V. KHARE, Department of Physics, University of Toledo, S.K.R. PATIL, Department of MIME, University of Toledo, N.M. MANGALE, Department of EECS, University of Toledo, S. MARSILLAC, Department of Physics, University of Toledo — We report a systematic study of mechanical and electronic properties of 32 cubic phases of nitrides of the transition metals M (M = Hf, Ta, W, Re, Os, Ir, Pt, Au), in zinc-blende, rocksalt, pyrite, and fluorite structure using *ab initio* computations. Our results reveal that MN_2(M = W, Re, Os, Ir, Pt, Au) in pyrite phase, have a bulk moduli greater than 330 GPa, MN_2(M = Re, Os, Ir) in fluorite phase have a bulk moduli greater than 350 GPa and TaN in rocksalt phase has a bulk modulus of 380 GPa making them candidates for super hardness. Based on the bulk and shear modulus for stable phases, potential hard coating materials for cutting tools have been identified. The local density of states of all phases has been obtained and linked to mechanical stability. The high values of bulk moduli are attributed to strong bonding of transition metal d-orbitals with nitrogen p-orbitals. The trend in the bulk modulus is related to the valence electron density of these materials.

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