Abstract Submitted
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Study the mechanical and magnetic properties of transition metal (M) nitrides in the cubic M4N structure using the first principle[1] INDIRAS KHATRI, V. ADHIKARI, S.V. KHARE, University of Toledo — We study the mechanical properties of twenty-eight transition metal (M) nitrides (TMNs) in metal-rich cubic M4N using the density functional theory [1]. We have computed lattice parameters, elastic constants, magnetic moments, formation energies, Debye temperature and Bader charge transfer. Our calculations indicate that all M4N-type nitrides except V4N, Nb4N, and Pt4N are mechanically stable. All Group 7 TMNs in the M4N structure are found to have high Vickers hardness values with the highest being 24.3 GPa for Re4N. Our computed lattice constants and magnetic dipole moments for Mn4N and Fe4N are consistent with their measured values. Spin-polarized computations reduce the hardness of some magnetic compounds like Mn4N and Fe4N. The hybridization of metal d and nitrogen 2p orbitals is found to be the key factor in determining mechanical stability and hardness in these compounds. In contrast, iconicity, as computed by Bader charge transfer, does not correlate with hardness. Our comprehensive database for binary M4N nitrides offers wide possibilities for experimental synthesis of such materials with desirable physical properties for the hard-coatings application. [1] V. Adhikari et. al., Journal of Physics and Chemistry of Solids, 120, 197, 2018

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