Abstract Submitted
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***Ab initio* calculations of MAX phases M_2TlC (M = Ti, Zr, Hf), and M_2GaN (M = Ti, V, Cr)** SANJAY KHARE, SUNIL PATIL, JACOB WARNER, Department of Physics, University of Toledo, Toledo, OH 43606 — MAX phases have been a subject of interest recently [cf. M. W. Barsoum Prog. Solid St. Chem. 28, 201 (2000).] because of their useful mechanical, electrical and thermal properties. Here we have studied two groups of M_2AX : (i) M = Ti, V, Cr, A = Ga and X = N and (ii) M = Ti, Zr, Hf, A = Tl and X = C. We calculated the lattice parameters, bulk modulus B and local electronic density of states (LDOS) of these phases using first-principles total energy calculations. Our computed lattice structural parameters match the experimental values within 5% for all six materials. Values for B were computed to be (i) 158, 170, and 180 GPa and (ii) 125, 120, and 131 GPa for the first and second group respectively. These values suggest that Ti_2TlC, Zr_2TlC and Hf_2TlC maybe the softest of all the MAX phases explored so far. The total density of states shows that all six materials are conducting. The major features in LDOS are i) the hybridization of the M d orbitals with X p orbitals and (ii) M d orbitals with A p orbitals.

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