# Supplementary material for: Density functional theory calculations of mechanical and electronic properties of $W_{1-x}Ta_xN_6$, $W_{1-x}Mo_xN_6$, and $Mo_{1-x}Ta_xN_6$ ($0 \leq x \leq 1$) alloys in hexagonal structure

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**Table S1**: Lattice constants ($a$, $c$), elastic constants ($C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$, and $C_{44}$), charge transfer per atom from metal to nitrogen ($Q_t$) in units of elementary charge $e$, and total magnetic moment (Mag.) in Bohr magneton ($\mu_B$) per transition metal atom for pure $MN_6$ compounds[1].

| Compounds | $a$ (Å) | $c$ (Å) | $C_{11}$ (GPa) | $C_{12}$ (GPa) | $C_{13}$ (GPa) | $C_{33}$ (GPa) | $C_{44}$ (GPa) | $Q_t$ ($e$) | Mag. ($\mu_B$) |
|---|---|---|---|---|---|---|---|---|---|
| $WN_6$ | 6.16 | 4.57 | 724 | 82 | 148 | 814 | 389 | 1.03 | 0 |
| $MoN_6$ | 6.18 | 4.58 | 677 | 99 | 145 | 736 | 354 | 1.09 | 0 |
| $TaN_6$ | 6.22 | 4.70 | 656 | 113 | 165 | 681 | 312 | 0.77 | 0 |

**Table S2**: Bulk modulus ($B$), shear modulus ($G$), Young's modulus ($E$), Vickers hardness ($H_V$), Pugh's ratio ($k$), Poisson's ratio ($\nu$), Debye temperature ($\theta_D$), formation energy per atom ($E_f$), and mass density ($\rho$) for pure $MN_6$ compounds[1].

| Compounds | $B$ (GPa) | $G$ (GPa) | $E$ (GPa) | $H_V$ (GPa) | $k$ | $\nu$ | $\theta_D$ (K) | $E_f$ (eV) | $\rho$ (kg/m$^3$) |
|---|---|---|---|---|---|---|---|---|---|
| $WN_6$ | 333 | 341 | 762 | 59 | 1.02 | 0.12 | 1048 | 1.03 | 8889 |
| $MoN_6$ | 317 | 309 | 699 | 52 | 0.97 | 0.13 | 1219 | 1.09 | 5928 |
| $TaN_6$ | 319 | 280 | 649 | 43 | 0.88 | 0.16 | 966 | 0.77 | 8381 |

**Fig. S1**: Relation between $\theta_D$ and a hardness parameter for all $M1_{1-x}M2_xN_6$ ($0 \leq x \leq 1$) compounds.

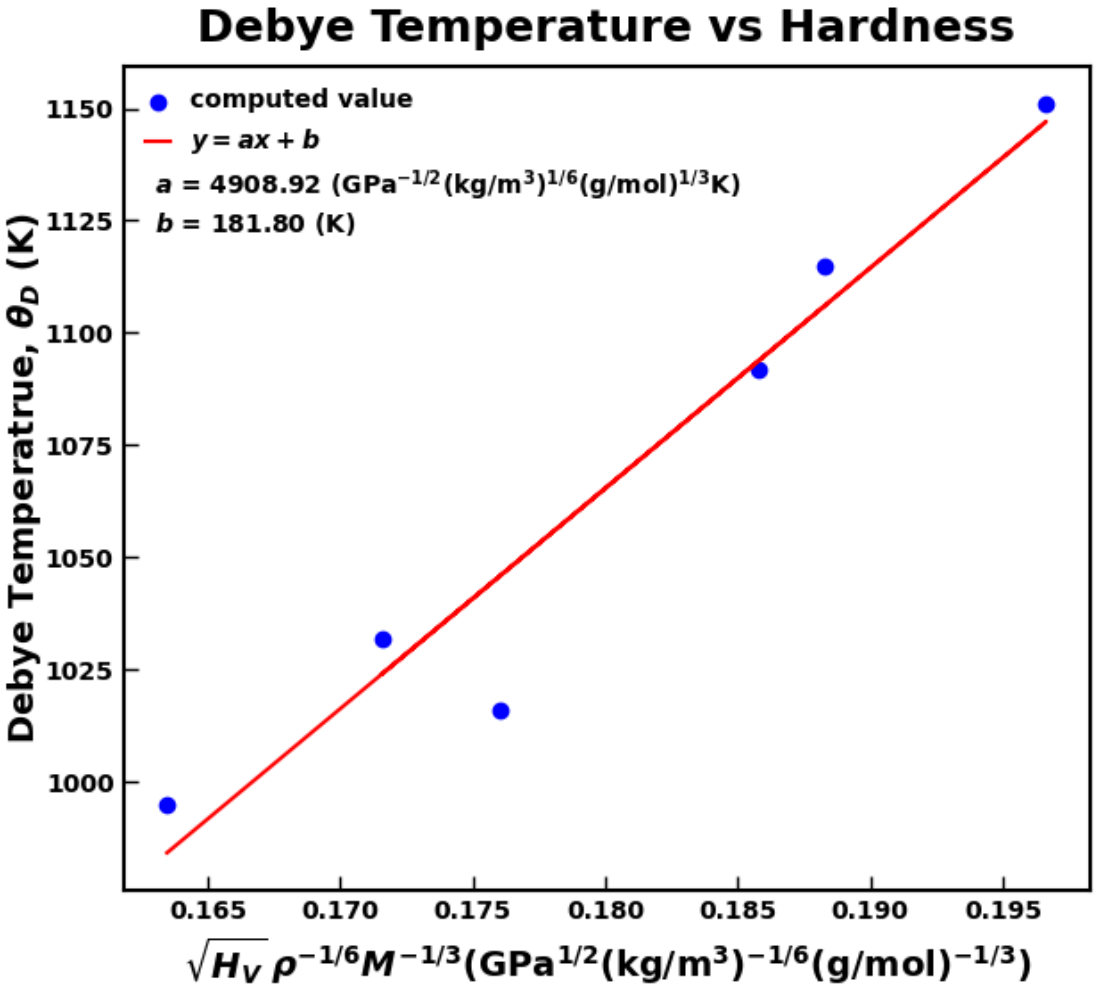
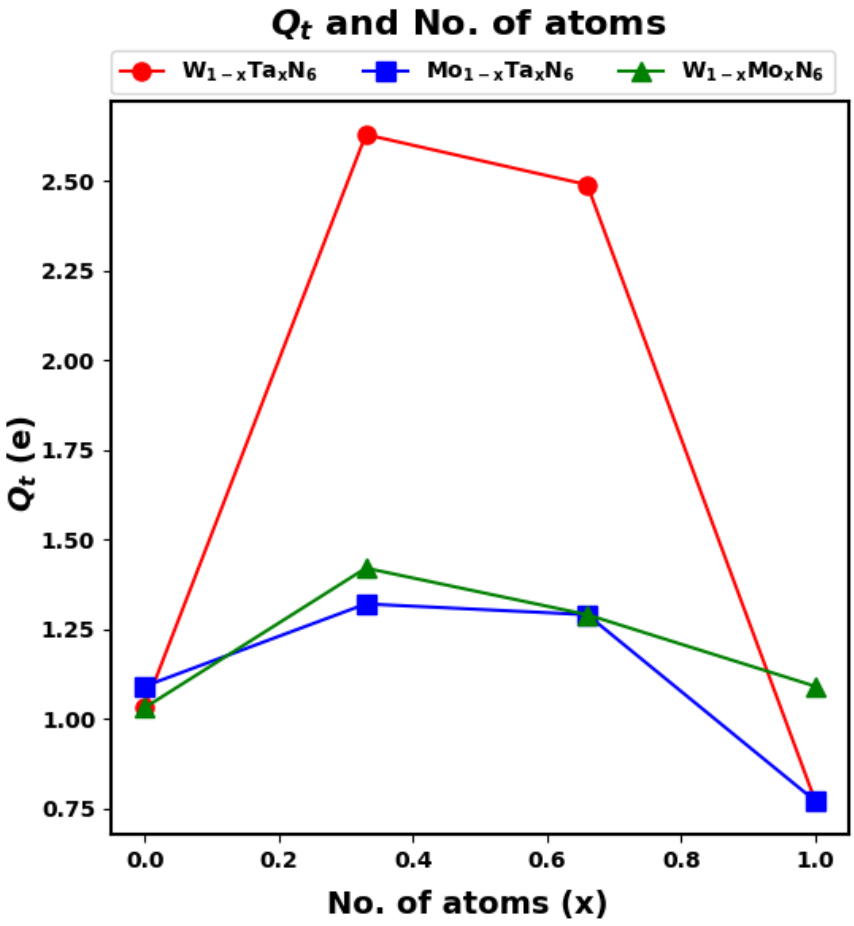


**Fig. S2**: Relation between $Q_t$ and number of atoms for all $M1_{1-x}M2_xN_6$ ($0 \leq x \leq 1$) compounds.



# References

1. S. R. Kandel, B. B. Dumre, D. Gall and S. V. Khare, Materialia **25**, 101550 (2022).