**Supporting Information**

# Versatile transition metals monolayers with Catalytic and Superconducting Properties: Computational study

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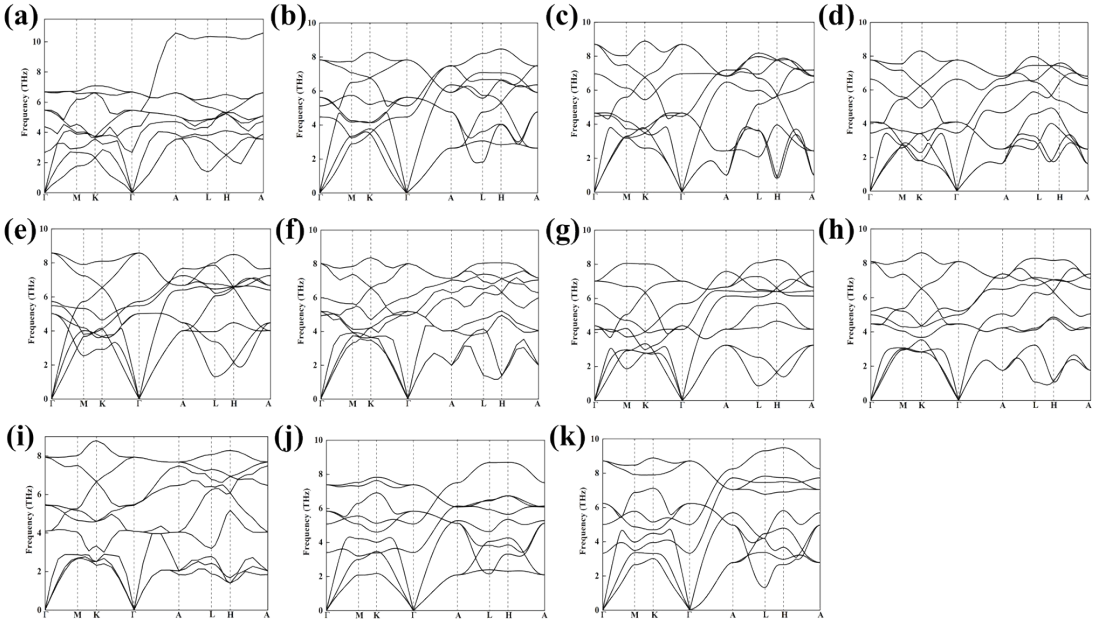


**Figure S1.** Phonon dispersion curves of (a) $TiRu_2$, (b) $VRu_2$, (c) $MnRu_2$, (d) $FeRu_2$, (e) $MoRu_2$, (f) $TcRu_2$, (g) $WRu_2$, (h) $ReRu_2$, (i) $OsRu_2$, (j) VOsRu, and (k) VFeRu.

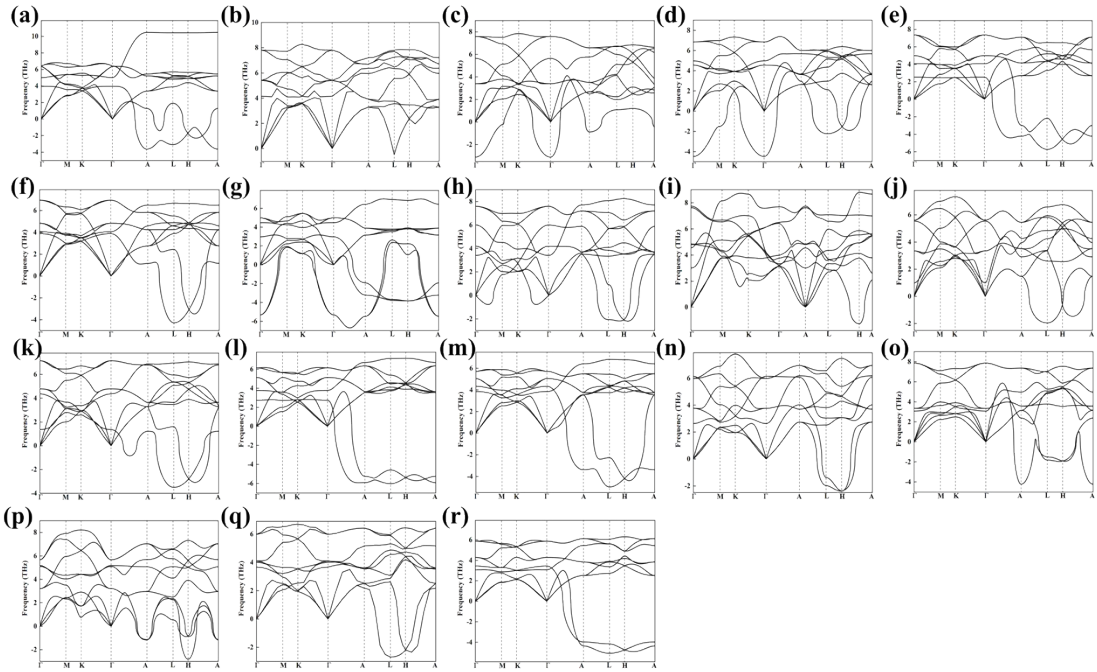


**Figure S2.** Phonon dispersion curves of (a) $ScRu_2$, (b) $CrRu_2$, (c) $CoRu_2$, (d) $NiRu_2$, (e) $CuRu_2$, (f) $ZnRu_2$, (g) $YRu_2$, (h) $ZrRu_2$, (i) $NbRu_2$, (j) $RhRu_2$, (k) $PdRu_2$, (l) $AgRu_2$, (m) $CdRu_2$, (n) $HfRu_2$, (o) $TaRu_2$, (p) $IrRu_2$, (q) $PtRu_2$ and (r) $AuRu_2$. It is clearly seen that phonon mode shows obvious softening in these systems, leading to structural instability.

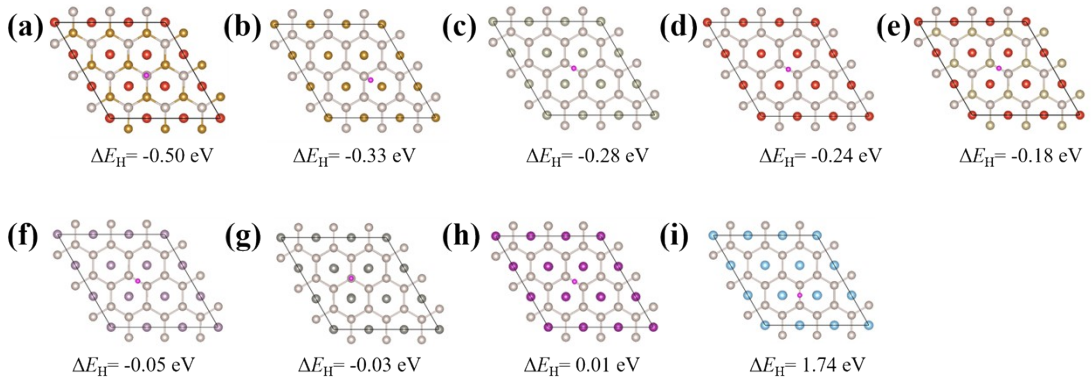


**Figure S3.** Optimized configurations for hydrogen atoms and Binding energies of VFeRu (a), $FeRu_2$ (b), $ReRu_2$ (c), $VRu_2$ (d), VOsRu (e), $MoRu_2$ (f), $WRu_2$ (g), $MnRu_2$ (h) and $TiRu_2$ (i).


**Figure S4.** Calculated *d*-band center among newly predicted compounds.

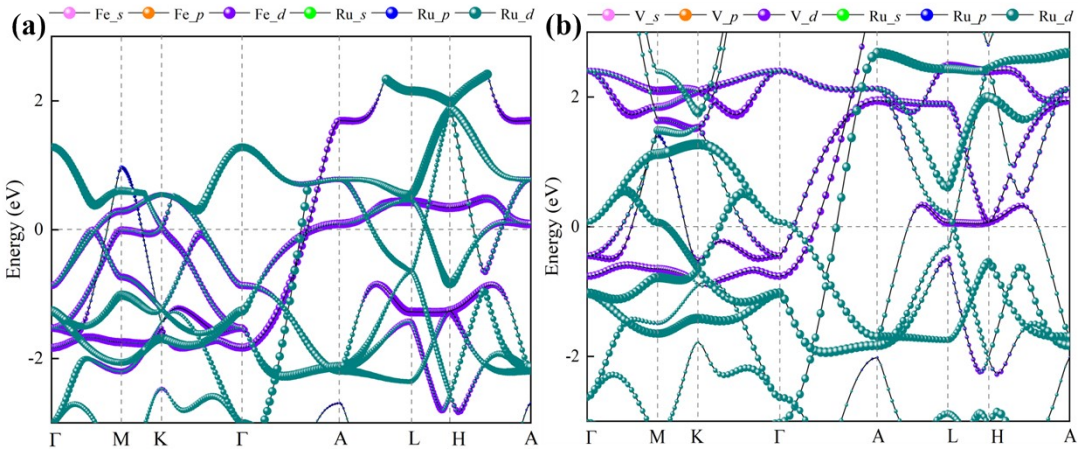


**Figure S5**. Calculated orbital-resolved band structures for (a) $FeRu_2$ and (b) $VRu_2$.

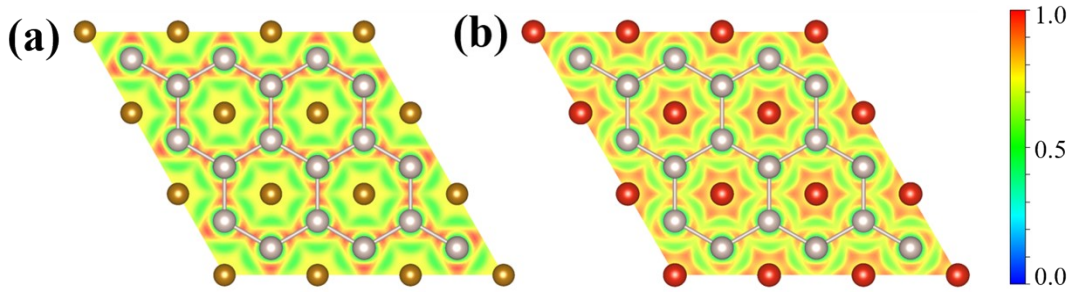


**Figure S6**. Electron localization function for $FeRu_2$ and $VRu_2$.

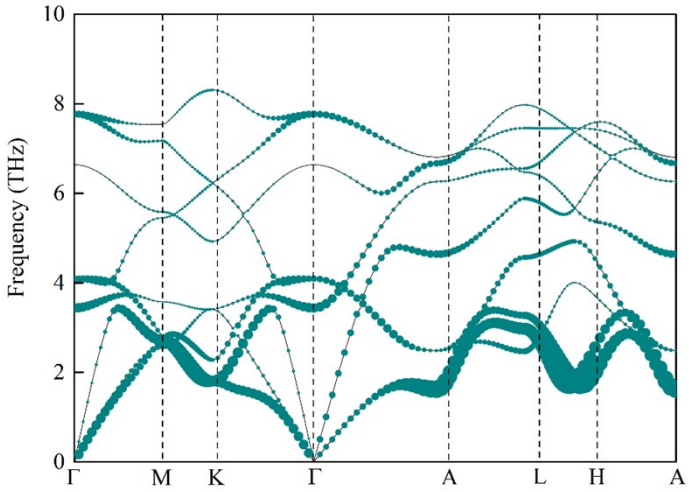


**Figure S7**. Calculated phonon band structure of $FeRu_2$ with the strength of $q$-resolved $\lambda_q$ indicated by circle size.

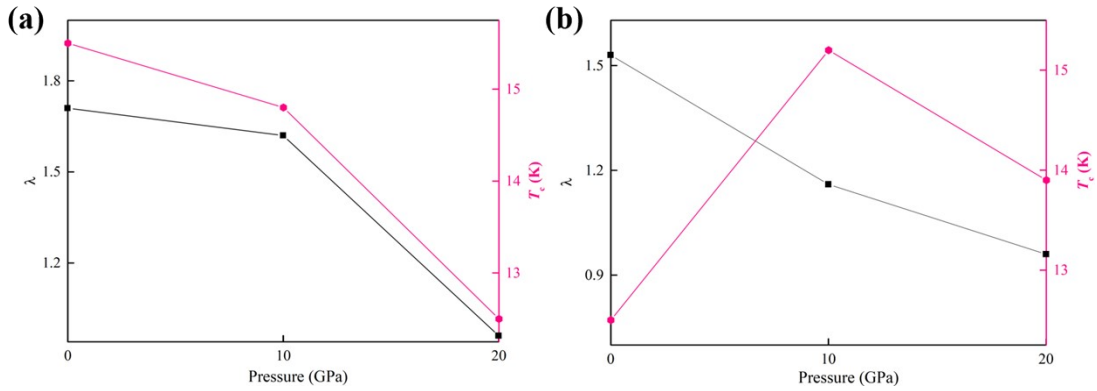


**Figure S8**. The variation of $T_c$, λ and pressure for (a) $FeRu_2$ and (b) VFeRu.

**Table S1**. Superconducting temperature (K) under different uniaxial and biaxial stresses. The percentages denote strains level which applied to transition metals monolayers.

| | uniaxial stresses | | | | biaxial stresses | | | |
|---|---|---|---|---|---|---|---|---|
| strain | +1% | +2% | -1% | -2% | +1% | +2% | -1% | -2% |
| $FeRu_2$ | 14.9 | 14.4 | 14.5 | 14.4 | 14.4 | 14.5 | 14.4 | 14.5 |
| $VRu_2$ | 12.8 | 12.7 | 12.8 | 12.8 | 12.8 | 12.8 | 12.8 | 12.8 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| $MnRu_2$ | 12.5 | 13.1 | 12.6 | 14.1 | 12.2 | 13.3 | 14.1 | 13.3 |
| $TiRu_2$ | 12.0 | 12.0 | 11.4 | 11.7 | 11.9 | 11.3 | 12.0 | 11.9 |
| $MoRu_2$ | 12.1 | 12.1 | 12.1 | 12.1 | 12.0 | 12.1 | 12.1 | 12.0 |
| $OsRu_2$ | 9.7 | 9.7 | 9.6 | 9.7 | 9.7 | 9.7 | 9.7 | 9.7 |
| $WRu_2$ | 8.7 | 8.8 | 8.8 | 8.8 | 8.8 | 8.7 | 8.7 | 8.7 |
| $TcRu_2$ | 7.7 | 7.7 | 7.7 | 7.7 | 7.7 | 7.7 | 7.7 | 7.6 |
| $ReRu_2$ | 6.2 | 6.2 | 6.2 | 6.2 | 6.2 | 6.2 | 6.2 | 6.2 |
| VFeRu | 12.6 | 12.7 | 14.8 | 16.0 | 14.2 | 16.1 | 15.9 | 13.7 |
| VOsRu | 9.0 | 9.0 | 9.0 | 8.8 | 8.9 | 9.0 | 8.9 | 8.9 |

**Table S2**. Calculated free energy of atomic hydrogen ($\Delta G_H$) and Binding energies ($\Delta E_H$) for different H atoms (n) adsorbed on an $VRu_2$ monolayer respectively.

| n | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|
| $\Delta G_H$ (eV) | -0.002 | 0.027 | 0.056 | 0.049 | 0.074 | 0.096 | 0.061 | 0.093 | 0.119 |
| $\Delta E_H$ (eV) | -0.242 | -0.213 | -0.184 | -0.191 | -0.166 | -0.144 | -0.179 | -0.147 | -0.121 |

**Table S3**. Calculated Bulk Modulus (B), Young's Modulus (E), and Shear Modulus (G) for stable $XRu_2$ (X= Ti, V, Mn, Fe, Mo, Tc, W, Re, Os) and VXRu (X=Os, Fe).

| $XRu_2$ | B (GPa) | E (GPa) | G (GPa) |
|---|---|---|---|
| $FeRu_2$ | 270 | 238 | 88 |
| $VRu_2$ | 254 | 198 | 726 |
| $MnRu_2$ | 280 | 286 | 107 |
| $TiRu_2$ | 218 | 131 | 468 |
| $MoRu_2$ | 281 | 285 | 107 |
| $OsRu_2$ | 325 | 395 | 152 |
| $WRu_2$ | 297 | 282 | 105 |
| $TcRu_2$ | 299 | 361 | 139 |
| $ReRu_2$ | 323 | 383 | 147 |
| VFeRu | 279 | 228 | 838 |
| VOsRu | 245 | 171 | 61 |

**Table S4**. Total energies (eV/atom) under different magnetic configurations.

| Configurations | NM | FM | AFM |
|---|---|---|---|
| $FeRu_2$ | -8.584 | -8.573 | -8.572 |
| $VRu_2$ | -9.134 | -9.134 | -9.135 |
| $MnRu_2$ | -8.918 | -8.918 | -8.894 |
| $TiRu_2$ | -8.910 | -8.910 | -8.911 |

| | | | |
|---|---|---|---|
| $MoRu_2$ | -9.671 | -9.671 | -9.671 |
| $OsRu_2$ | -9.656 | -9.656 | -9.655 |
| $WRu_2$ | -10.317 | -10.317 | -10.317 |
| $TcRu_2$ | -9.479 | -9.479 | -9.479 |
| $ReRu_2$ | -10.148 | -10.148 | -10.148 |
| VFeRu | -8.725 | -8.725 | -8.725 |
| VOsRu | -9.743 | -9.743 | -9.743 |