# Supplementary Information

# First-principles study of structural, electronic, elastic, and high-pressure properties of $(V_{2/3}Zr_{1/3})_2AlC$ *i*-MAX phase and $M_2AlC$ (M = V, Zr) MAX phases

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**Table S1 The calculated Bader charges (e) of all the constituent elements of $M_2AlC$ (M = V, Zr) MAX phases and $(V_{2/3}Zr_{1/3})_2AlC$ *i*-MAX phase. Comparison with previously published data is also included.**

| System | Bader Charges (e) | | | | | | |
|---|---|---|---|---|---|---|---|
| | Zr1 | V1 | V2 | Al1 | Al2 | C1 | C2 |
| $V_2AlC$ | — | 0.978 | | -0.27 | | -1.683 | |
| $Zr_2AlC$ | 1.44 | — | | -0.810 | | -2.077 | |
| Ref [1] | 1.443 | | | -0.812 | | -2.074 | |
| $(V_{2/3}Zr_{1/3})_2AlC$ | 1.471 | 0.960 | 0.961 | -0.455 | -0.516 | -1.782 | -1.758 |

**Table S2 Calculated net atomic charges, NAC (e) of all the constituent elements of $M_2AlC$ (M = V, Zr) MAX phases and $(V_{2/3}Zr_{1/3})_2AlC$ *i*-MAX phase.**

| System | NAC (e) | | | | | | |
|---|---|---|---|---|---|---|---|
| | Zr1 | V1 | V2 | Al1 | Al2 | C1 | C2 |
| $V_2AlC$ | — | 0.749 | | -0.217 | | -1.282 | |
| $Zr_2AlC$ | 0.972 | — | | -0.523 | | -1.422 | |
| $(V_{2/3}Zr_{1/3})_2AlC$ | 0.907 | 0.733 | 0.732 | -0.262 | -0.268 | -1.322 | -1.312 |

**Table S3 The calculated sum of bond order, SBO (e), of all the constituent elements of $M_2AlC$ (M = V, Zr) MAX phases and $(V_{2/3}Zr_{1/3})_2AlC$ *i*-MAX phase.**

| System | Sum of bond order (SBO) (e) | | | | | | |
|---|---|---|---|---|---|---|---|
| | Zr1 | V1 | V2 | Al1 | Al2 | C1 | C2 |
| $V_2AlC$ | — | 4.034 | | 3.426 | | 4.673 | |
| $Zr_2AlC$ | 3.992 | — | | 3.053 | | 4.185 | |
| $(V_{2/3}Zr_{1/3})_2AlC$ | 3.817 | 4.076 | 4.077 | 3.601 | 3.637 | 4.536 | 4.463 |

**Table S4 The calculated atomic basin volume (Å$^3$) of all the elemental species of $M_2AlC$ (M = V, Zr) MAX phases and $(V_{2/3}Zr_{1/3})_2AlC$ *i*-MAX phase.**

| System | Atomic basin volume (Å$^3$) | | | | | | |
|---|---|---|---|---|---|---|---|
| | Zr1 | V1 | V2 | Al1 | Al2 | C1 | C2 |
| $V_2AlC$ | — | 70.39 | | 113.06 | | 69.59 | |
| $Zr_2AlC$ | 101.74 | — | | 170.14 | | 95.70 | |
| $(V_{2/3}Zr_{1/3})_2AlC$ | 98.52 | 71.52 | 71.50 | 120.16 | 121.12 | 76.80 | 77.04 |

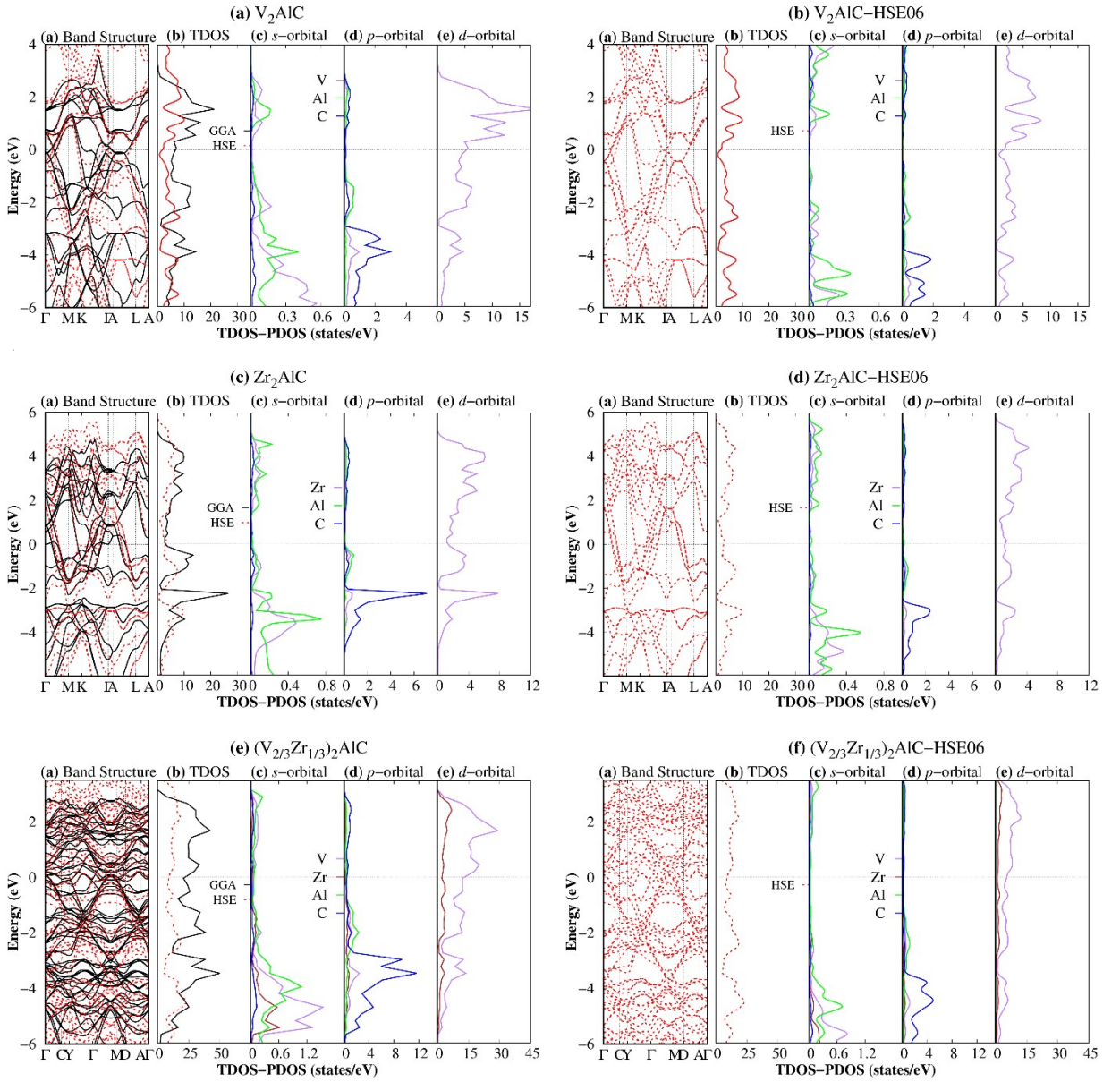


**Figure S1 The band structure, total density of states, and partial density of states for (a-b) $V_2AlC$, (c-d) $Zr_2AlC$, and (e-f) $(V_{2/3}Zr_{1/3})_2AlC$. In Figures (a, c, d), the solid black lines represent the band structure and total density of states (TDOS) calculated via GGA, while the dotted red lines represent the band structure and TDOS calculated via HSE06.**

## **References**:

[1] S.H. Shah, P.D. Bristowe, Point defect formation in M2AlC (M = Zr,Cr) MAX phases and their tendency to disorder and amorphize, Sci. Rep. 7 (2017) 9667. https://doi.org/10.1038/s41598-017-10273-6.