Supplementary Information

DFT insights into the electronic structure, mechanical behaviour, lattice dynamics and defect processes in the first Sc-based MAX phase Sc2SnC

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**Table** **S1**. Lattice parameters (*a*, *c*, *z*M in Å), hexagonal ratio (*c*/*a*) and cell volume (*V* in Å3) of Sc2SnC and existing M2SnC MAX phases.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound | *a* | *c* | *c*/*a* | *z*M | *V* | Remarks |
| Sc2SnC | 3.373 | 14.854 | 4.403 | 0.5814 | 146.4 | Calc.This |
|  | 3.368 | 14.653 | 4.351 | 0.5786 | 143.9 | Expt.1 |
| V2SnC | 3.121 | 12.947 | 4.148 | 0.0759 | 109.2 | Calc.2 |
| 2.9792 | 13.4441 | 4.513 | 0.0744 | 103.3 | Expt.3 |
| Ti2SnC | 3.172 | 13.772 | 4.342 | 0.0806 | 120.0 | Calc.4 |
| 3.1635 | 13.675 | 4.323 | --------- | 118.5 | Expt.5 |
| Nb2SnC | 3.258 | 13.918 | 4.272 | 0.0820 | 128.0 | Calc.4 |
| 3.2408 | 13.802 | 4.259 | --------- | 125.5 | Expt.5 |
| Hf2SnC | 3.367 | 14.548 | 4.320 | 0.0865 | 142.9 | Calc.4 |
| 3.3199 | 14.388 | 4.334 | --------- | 137.3 | Expt.5 |
| Zr2SnC | 3.367 | 14.730 | 4.374 | 0.0849 | 144.7 | Calc.4 |
| 3.3576 | 14.568 | 4.339 | --------- | 142.2 | Expt.5 |
| Lu2SnC | 3.546 | 15.323 | 4.320 | 0.0850 | 166.9 | Calc.4 |
| 3.514 | 15.159 | 4.314 | --------- | 162.1 | Expt.5 |

**Table S2**. Effective valence charge, bond population and bond length of M2SnC MAX phases

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Sc2SnC | Ti2SnC | V2SnC | Zr2SnC | Nb2SnC | Lu2SnC | Hf2SnC |
| Atom | Effective valence charge (e) | | | | | | |
| M | 2.47 | 3.58 | 3.68 | 3.57 | 4.69 | 2.55 | 3.72 |
| Sn | 3.79 | 3.89 | 3.99 | 3.93 | 3.93 | 3.54 | 3.69 |
| C | 3.15 | 3.22 | 3.36 | 3.22 | 3.32 | 3.57 | 3.14 |
| Bond | Bond population | | | | | | |
| M-C | 1.17 | 1.08 | 1.02 | 1.05 | 0.99 | –6.25 | 1.39 |
| M-M | –0.52 | –0.34 | –0.42 | –0.09 | –0.26 | –3.62 | –0.31 |
| M-Sn | 0.14 | –0.35 | –0.35 | –0.66 | –1.03 | –1.16 | –0.16 |
| Sn-C | –0.13 | –0.13 | –0.18 | –0.05 | –0.05 | 0.12 | –0.19 |
| Bond | Bond length (Å) | | | | | | |
| M-C | 2.293 | 2.141 | 2.053 | 2.312 | 2.200 | 2.428 | 2.316 |
| M-M | 3.106 | 2.878 | 2.667 | 3.168 | 2.958 | 3.314 | 3.180 |
| M-Sn | 3.172 | 2.966 | 2.886 | 3.113 | 3.001 | 3.255 | 3.071 |
| Sn-C | 4.193 | 3.900 | 3.705 | 4.163 | 3.955 | 4.345 | 4.123 |

**Table S3**. Elastic constants *C*ij and moduli *B*, *G*, *E* in GPa and Poisson’s and Pugh’s ratio *v* and *B*/*G* of Sc2SnC including M2SnC2,4.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Phases | *C*11 | *C*33 | *C*44 | *C*66 | *C*12 | *C*13 | *B* | *G* | *E* | *v* | *B*/*G* |
| Sc2SnC | 187 | 184 | 61 | 64 | 59 | 43 | 94 | 65 | 158 | 0.220 | 1.455 |
| Ti2SnC | 268 | 265 | 100 | 95 | 79 | 74 | 139 | 97 | 236 | 0.213 | 1.406 |
| V2SnC | 243 | 300 | 87 | 84 | 76 | 124 | 156 | 82 | 209 | 0.278 | 1.914 |
| Zr2SnC | 230 | 232 | 94 | 84 | 62 | 91 | 131 | 83 | 206 | 0.236 | 1.560 |
| Nb2SnC | 255 | 236 | 94 | 77 | 102 | 122 | 160 | 78 | 217 | 0.280 | 1.944 |
| Lu2SnC | 172 | 173 | 56 | 64 | 46 | 36 | 82 | 61 | 152 | 0.206 | 1.370 |
| Hf2SnC | 251 | 238 | 101 | 90 | 71 | 107 | 145 | 87 | 216 | 0.252 | 1.681 |

**Table S4**. Elastic anisotropy factors of Sc3SnC including existing M2SnC2,4 MAX phases.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Phases | *A*1 | *A*2 | *A*3 | *k*c/*k*a | *AB%* | *AG%* | *AU* |
| Sc2SnC | 1.2077 | 0.9531 | 1.1510 | 1.1348 | 0.1085 | 0.2482 | 0.0271 |
| Ti2SnC | 0.9683 | 1.0582 | 1.0247 | 1.0419 | 0.0011 | 0.0284 | 0.0025 |
| V2SnC | 0.8103 | 1.0419 | 0.8443 | 0.4034 | 1.8476 | 0.7283 | 0.1110 |
| Zr2SnC | 0.6950 | 1.1190 | 0.7778 | 0.7801 | 0.2353 | 1.0100 | 0.1067 |
| Nb2SnC | 0.6046 | 1.2288 | 0.7429 | 0.9912 | 0.0926 | 1.4360 | 0.1475 |
| Lu2SnC | 1.2500 | 0.8889 | 1.1111 | 1.0657 | 0.0068 | 0.4086 | 0.0412 |
| Hf2SnC | 0.6106 | 1.1222 | 0.6852 | 0.8244 | 0.1637 | 1.5501 | 0.1607 |

**Table** **S5.** Bond number *nμ*, bond length, *d*μ (Å), bond population *P*μ, bond volume (Å3), bond hardness (GPa), metallic population *P*μ′, and hardness (GPa) of Sc2SnC and existing M2SnC MAX phases.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Compound | Bond | *n*μ | *d*μ | *P*μ | *P*μ′ |  |  | *H*V | *H*V (expt.) |
| Sc2SnC | Sc-C | 4 | 2.2927 | 1.17 | 0.00568 | 36.60 | 2.1 | 2.1 |  |
| Ti2SnC | Ti–C | 4 | 2.1414 | 1.08 | 0.01525 | 30.00 | 2.7 | 2.7 | 3.55, 3.56 |
| V2SnC | V–C | 4 | 2.0526 | 1.02 | 0.05432 | 27.30 | 2.9 | 2.9 |  |
| Zr2SnC | Zr–C | 4 | 2.3118 | 1.05 | 0.01302 | 36.18 | 1.9 | 1.9 | 3.55, 3.96 |
| Nb2SnC | Nb–C | 4 | 2.2014 | 0.99 | 0.00139 | 31.98 | 2.3 | 2.3 | 3.86, 3.56 |
| Lu2SnC | Sn–C | 4 | 4.3478 | 0.12 | 0.00348 | 41.82 | 0.2 | 0.2 |  |
| Hf2SnC | Hf–C | 4 | 2.3158 | 1.39 | 0.00541 | 35.73 | 2.6 | 2.6 | 3.85, 4.56 |

**Table S6**. Sound velocities in km/s, Debye temperature and melting point in K, minimum and room temperature lattice thermal conductivity in W/m-K of Sc2SnC and existing M2SnC2,4 MAX phases.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Phases | *ρ* | *vl* | *vt* | *vm* | *θ*D | *T*m |  | *κ*ph\* |
| Sc2SnC | 5.005 | 6.004 | 3.596 | 3.978 | 449 | 1191 | 0.79 | 09.60 |
| Ti2SnC | 6.346 | 6.503 | 3.910 | 4.325 | 525 | 1556 | 0.99 | 29.98 |
| V2SnC | 7.073 | 6.125 | 3.405 | 3.792 | 472 | 1533 | 1.20 | 14.38 |
| Zr2SnC | 7.313 | 5.749 | 3.369 | 3.735 | 426 | 1392 | 0.76 | 20.61 |
| Nb2SnC | 8.369 | 5.616 | 3.053 | 3.469 | 412 | 1473 | 0.76 | 12.38 |
| Lu2SnC | 9.847 | 4.073 | 2.489 | 2.748 | 300 | 1130 | 0.51 | 14.91 |
| Hf2SnC | 11.796 | 4.704 | 2.716 | 3.015 | 348 | 1464 | 0.63 | 15.92 |

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