**Electronic Supplemental Materials (ESM)**

**The site preference and doping effect on mechanical properties of Ni3Al-based γ′ phase in superalloys by combing first-principles calculations and thermodynamic model**

Hamid Alia, Rong Chena, Bo Wua, b, \*, Tianliang Xiea, Liangji Wenga, Jiansen Wena, Qipeng Yaoa, Longju Sua, Yan Zhaoa, Panhong Zhaob, Baisheng Saa, Yu Liuc, ChunxuWangc, Hang Suc, Asif Hayatd, e, \*

*aMultiscale Computational Materials Facility, Key Laboratory of Eco-Materials Advanced Technology, College of Materials Science and Engineering, Fuzhou University, Fuzhou 350100, China*

*bMaterials Design and Manufacture Simulation Facility, School of Advance Manufacturing, Fuzhou University, Jinjiang 362200, China.*

*cCentral Iron & Steel Research Institute Group, Beijing, 100081, China.*

*dCollege of Chemistry and Life Sciences, Zhejiang Normal University, Jinhua 321004, Zhejiang PR, China.*

*eCollege of Geography and Environmental Sciences, Zhejiang Normal University, Jinhua, 321004, China.*

**\*Corresponding authors**

[wubo@fzu.edu.cn](mailto:wubo@fzu.edu.cn), [asifncp11@yahoo.com](mailto:asifncp11@yahoo.com)

**Table S1.** The supercell dimension and the Brillouin zone sampling (KPOINTS) of the different types of pure elements and end-members involved in this study.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Element/  End-members | Structure (SER) | Structure relaxation | | Phonon calculation | |
| Atoms in primitive cell （POSCAR） | Brillouin zone sampling (KPOINTS) | Supercell dimension | Brillouin zone sampling (KPOINTS) |
| Al | FCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| Co | HCP | 2 | Gamma  8×8×6 | 2×2×1 | Gamma  4×4×3 |
| Cr | BCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| Cu | FCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| Fe | BCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| Mn | BCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| Mo | BCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| Ni | FCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| Re | HCP | 2 | Gamma  8×8×6 | 2×2×1 | Gamma  4×4×3 |
| Ta | BCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| Ti | HCP | 2 | Gamma  8×8×6 | 2×2×1 | Gamma  4×4×3 |
| V | BCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| W | BCC | 1 | Monkhorst-Pack 10×10×10 | 2×2×2 | Monkhorst-Pack 10×10×10 |
| AB3\_L12 | L12 (ordered FCC) | 4 | Monkhorst-Pack  6×6×6 | 2×2×2 | Monkhorst-Pack  6×6×6 |

**Table S2.** The fundamental information of structures and properties of stable elements at room temperature involved in this study.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Elements | Stable structure | Space | Space | Atomic weight | χ | Molecular weight | Density | Melting point | Boiling point | Molar volume | Bulk modulus | Shear modulus | Young modulus | Poisson ratio |
| No. | group | g/mol | g/cm3 | K | K | cm3/mol | B (GPa) | G (GPa) | E (GPa) | ν |
| Al | FCC\_A1 | 225 | Fm\_3m | 26.98 | 1.61 | 26.98 | 2.70 | 933 | 2792 | 9.99 | 76 | 26 | 70 | 0.35 |
| Co | HCP\_A3 | 194 | P63/mmc | 58.93 | 1.88 | 58.93 | 8.90 | 1768 | 3200 | 6.62 | 180 | 76 | 209 | 0.31 |
| Cr | BCC\_A2 | 229 | Im\_3m | 52.00 | 1.66 | 52.00 | 7.19 | 2180 | 2944 | 7.28 | 160 | 115 | 279 | 0.21 |
| Cu | FCC\_A1 | 225 | Fm\_3m | 63.55 | 1.90 | 63.55 | 8.96 | 1357 | 2835 | 7.11 | 140 | 48 | 130 | 0.34 |
| Fe | BCC\_A2 | 229 | Im\_3m | 55.85 | 1.83 | 55.85 | 7.87 | 1811 | 3134 | 7.09 | 170 | 82 | 211 | 0.29 |
| Mn\* | BCC\_A2 | 217 | l\_43m | 54.94 | 1.55 | 54.94 | 7.47 | 1519 | 2334 | 7.39 | 120 | 76 | 198 | 0.35 |
| Mo | BCC\_A2 | 229 | lm\_3m | 42.00 | 2.16 | 95.94 | 10.22 | 2890 | 4885 | 9.41 | 261 | 120 | 324 | 0.29 |
| Ni | FCC\_A1 | 225 | Fm3m | 58.69 | 1.91 | 58.69 | 8.91 | 1728 | 3186 | 6.58 | 180 | 76 | 200 | 0.31 |
| Re | HCP\_A3 | 194 | P63/mmc | 186.21 | 1.90 | 186.21 | 21.02 | 3459 | 5869 | 8.86 | 370 | 178 | 463 | 0.30 |
| Ta | BCC\_A2 | 229 | Im\_3m | 180.96 | 1.50 | 180.95 | 16.65 | 3290 | 5731 | 10.86 | 200 | 67 | 186 | 0.34 |
| Ti | HCP\_A3 | 194 | P63/mmc | 47.87 | 1.62 | 47.87 | 4.507 | 1941 | 3560 | 10.54 | 110 | 44 | 116 | 0.32 |
| V | BCC\_A2 | 229 | Im\_3m | 50.94 | 1.63 | 50.94 | 6.11 | 2183 | 3680 | 8.33 | 160 | 47 | 128 | 0.37 |
| W | BCC\_A2 | 229 | Im\_3m | 183.84 | 2.36 | 183.84 | 19.25 | 3695 | 5828 | 9.55 | 310 | 161 | 411 | 0.28 |

\*here we simply chose Mn\_BCC as SER, due to Mn-CBCC-A12 containing 48 atoms in a unit cell, which involve considerable large computing time for QHA-thermal properties.

**Table S3.**  Lattice constant and bulk modulus B0 of pure elements.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Element | Lattice Constant, Å | | | B0, GPa | | |
| This work | Others work | Ref. | This work | Others work | Ref. |
| Al\_FCC | a=4.04 | a=4.05 | **[1]** | 80 | 78 | **[2]** |
| Co\_HCP | a=2.49  c/a=1.63 | a=2.49  c/a=1.61 | **[1]** | 217 | 191  205 | **[3]**  **[4]** |
| Cr\_BCC | a=2.837 | a=2.847 | **[1]** | 260 | 190  283 | **[3]**  **[5]** |
| Cu\_FCC | a=3.60 | A=3.63 | **[1]** | 168 | 141 | **[2]** |
| Fe\_BCC | a=2.83 | a=2.82 | **[1]** | 189 | 168 | **[3]** |
| Mn\_BCC | a=2.78 | A=2.79 | **[1]** | 272 | 276 | **[2]** |
| Mo\_BCC | a=3.10 | a=3.16 | **[6]** | 267 | 260 | **[6]** |
| Ni\_FCC | a=3.53 | a=3.52 | **[1]** | 196 | 185 | **[3]** |
| Re\_HCP | a=2.70  c/a=1.62 | a=2.78  c/a=1.62 | **[6]** | 378 | 367 | **[6]** |
| Ta\_BCC | a=3.28 | a=3.32 | **[6]** | 163 | 199 | **[6]** |
| Ti\_HCP | a=2.94  c/a=1.56 | a=2.93  c/a=1.58 | **[1]** | 117 | 105 | **[3]** |
| V\_BCC | a=2.96 | A=2.99 | **[1]** | 174 | 160 | **[2]** |
| W\_BCC | a=3.15 | a=3.18 | **[6]** | 316 | 306 | **[6]** |

**Table S4.** Calculated total energy of pure elements at ground state (0 K).

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Elements | Etot (eV/atom) | Etot J/(mol·atom) | Elements | Etot (eV/atom) | Etot J/(mol·atom) | Elements | Etot (eV/atom) | Etot J/(mol·atom) |
| Al\_FCC | -3.7155 | -358489.0430 | Fe\_BCC | -8.3128 | -802064.2709 | Re\_HCP | -11.9950 | -1157339.9030 |
| Co\_HCP | -7.1082 | -685831.3483 | Mn\_BCC | -8.8669 | -855525.1621 | Ta\_BCC | -11.3281 | -1092995.2020 |
| Cr\_BCC | -9.5196 | -918498.5578 | Mo\_BCC | -10.7300 | -1035282.8440 | Ti\_HCP | -7.7625 | -748966.6095 |
| Cu\_FCC | -3.7097 | -357931.0799 | Ni\_FCC | -5.5779 | -538183.1508 | V\_BCC | -8.9226 | -860893.7323 |
|  |  |  |  |  |  | W\_BCC | -11.1695 | -1077687.1330 |

**Table S5.** Calculated, in (eV/atom), *∆Hf* in (J/mol.atom) at ground state (0 K), and *∆G* in (J/mol.atom) at different temperatures of all end-members (A)1a (B)3c.

|  |  | Etot | ∆Hf | ∆G300K | ∆G1000K |  |  | Etot | ∆Hf | ∆G300K | ∆G1000K |  |  | Etot | ∆Hf | ∆G300K | ∆G1000K |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Al | Al | -3.7260 | -1016.9857 | -100.0000 | -100.0000 | Fe | Fe | -8.1562 | 15109.1409 | 12733.0219 | 9277.0215 | Re | Re | -12.0698 | -7217.1865 | 5348.2285 | 10638.8832 |
| Al | Co | -6.4587 | -19169.2683 | -17728.3310 | -18134.4070 | Fe | Mn | -8.7656 | -3593.2702 | 55180.7577 | 49026.1682 | Re | Ta | -11.8017 | -29610.3269 | 14677.0971 | 17247.9889 |
| Al | Cr | -7.9029 | 15987.7671 | 13327.3213 | 15038.6962 | Fe | Mo | -9.9616 | 15829.3170 | 29664.1195 | 26041.8014 | Re | Ti | -8.9150 | -9104.8794 | -1670.3567 | -2915.1226 |
| Al | Cu | -3.9190 | -20049.9472 | -3962.4845 | -2921.6349 | Fe | Ni | -6.0944 | 16135.0056 | -10733.8235 | -11652.1219 | Re | V | -9.6144 | 7364.3050 | 11356.5956 | 12136.4127 |
| Al | Fe | -7.3757 | -20477.8823 | -17863.9571 | -12851.5267 | Fe | Re | -11.2606 | -17961.9280 | 92392.3726 | 84012.0709 | Re | W | -12.2378 | -83161.4678 | 28252.6420 | 20250.4196 |
| Al | Mn | -7.7159 | -13205.3013 | -11515.2090 | -14623.3345 | Fe | Ta | -10.7091 | -13008.6866 | 21333.9597 | 23031.7704 | Ta | Al | -5.9086 | -27977.2561 | -16597.2534 | -22567.4140 |
| Al | Mo | -9.0573 | -7808.0149 | 5328.6721 | -265.8324 | Fe | Ti | -7.8244 | 7302.1024 | 4165.4973 | 564.1366 | Ta | Co | -8.5370 | -36072.1354 | -24764.9235 | -26389.1579 |
| Al | Ni | -5.5585 | -43056.1080 | -40096.8899 | -31684.3858 | Fe | V | -8.6091 | 15535.4237 | 11878.6821 | 15749.8873 | Ta | Cr | -9.6327 | 32714.7951 | 36063.4121 | 20963.8045 |
| Al | Re | -9.9420 | -1629.0461 | 14924.8478 | 2337.5862 | Fe | W | -11.4838 | -99234.4969 | 28102.6123 | 21096.3797 | Ta | Cu | -5.3821 | 22400.5606 | 27480.4508 | 24597.3886 |
| Al | Ta | -9.8797 | -43878.6788 | -9671.2440 | -12532.8667 | Mn | Al | -5.2114 | -20072.3366 | -9244.9609 | -12907.3598 | Ta | Fe | -9.1749 | -10444.2842 | -4629.9660 | -8439.0157 |
| Al | Ti | -7.0188 | -25860.1081 | -27422.3529 | -30635.8731 | Mn | Co | -7.5470 | 831.2304 | 7731.3902 | 6733.3855 | Ta | Mn | -9.1749 | 29651.3843 | 3177.6866 | -2253.3829 |
| Al | V | -7.6974 | -7387.9192 | -11235.9917 | -21276.7115 | Mn | Cr | -9.0955 | 25172.6832 | 18736.2533 | 9891.4543 | Ta | Mo | -10.7660 | 10952.5310 | 38011.0591 | 46074.8972 |
| Al | W | -10.4759 | -11288.2191 | 14326.1601 | 5743.9516 | Mn | Cu | -4.5820 | 40237.8391 | 36269.2231 | 35812.4221 | Ta | Ni | -7.3161 | -29007.9620 | -21462.4742 | -21512.1629 |
| Co | Al | -4.8021 | -23001.7538 | -20264.0023 | -18272.9262 | Mn | Fe | -8.3669 | 8147.4105 | 6549.4872 | 3063.8163 | Ta | Re | -12.1842 | -34336.1803 | 3262.7734 | -5487.1636 |
| Co | Co | -7.0928 | 1481.4307 | -3868.6046 | -11808.5524 | Mn | Mn | -8.9439 | -7426.4022 | -85321.7137 | -88641.4416 | Ta | Ta | -11.6092 | -27120.4621 | 19653.2802 | 18560.9744 |
| Co | Cr | -8.7256 | 18444.8927 | 9740.8145 | -163.1578 | Mn | Mo | -10.0394 | 21695.3156 | 31135.0649 | 29790.3700 | Ta | Ti | -8.6908 | -3556.8019 | 6944.7593 | 935.7244 |
| Co | Cu | -4.3666 | 18594.7219 | 12655.1644 | 12951.2602 | Mn | Ni | -6.5436 | -13843.4869 | 11483.3486 | 15408.4039 | Ta | V | -9.3774 | 14142.1803 | 23338.6050 | 25110.3718 |
| Co | Fe | -7.2115 | 77206.1030 | 12412.3565 | 17127.4745 | Mn | Re | -11.4179 | -19766.9211 | -1017.4955 | -10016.5233 | Ta | W | -12.2588 | -10127.6391 | 41071.2967 | 40659.6876 |
| Co | Mn | -6.8426 | 15289.0638 | -7138.4026 | -12235.3821 | Mn | Ta | -10.8385 | -12129.3706 | 23303.3506 | 25328.9644 | Ti | Al | -5.1117 | -37091.3170 | -38221.7011 | -43028.5574 |
| Co | Mo | -9.7804 | 4259.5715 | 18752.4986 | 13845.9528 | Mn | Ti | -7.9451 | 9020.2590 | 8521.9899 | 8341.2489 | Ti | Co | -7.5228 | -24225.9155 | -24954.9211 | -28269.3254 |
| Co | Ni | -6.7219 | -73465.2228 | -767.9462 | -1752.9943 | Mn | V | -8.7286 | 17372.2810 | 14326.1776 | 16958.0580 | Ti | Cr | -8.6510 | 41421.1519 | 34370.7926 | 35274.3512 |
| Co | Re | -11.0748 | -29087.0465 | -6131.5469 | -17775.7511 | Mn | W | -11.5315 | -90465.3612 | 27318.0755 | -6836.6677 | Ti | Cu | -1.2256 | 33743.4647 | 4633.7125 | -1373.2718 |
| Co | Ta | -10.5113 | -22980.2305 | 11849.2178 | 11398.2476 | Mo | Al | -5.6353 | -16035.2233 | -11408.6238 | -17073.3026 | Ti | Fe | -8.2385 | -6104.0666 | -12297.5414 | -20362.8976 |
| Co | Ti | -7.6152 | -1574.1679 | -4730.6722 | -7166.6849 | Mo | Co | -8.0676 | -5208.3809 | -2377.3621 | -22121.6341 | Ti | Mn | -8.5489 | 4043.6950 | -6172.0562 | -13056.8802 |
| Co | V | -8.4014 | 6522.0242 | 3726.5018 | 4843.3208 | Mo | Cr | -9.3780 | 42857.8169 | 35519.7735 | 29800.4147 | Ti | Mo | -9.7799 | 20086.1233 | 15463.0853 | 15129.8756 |
| Co | W | -11.2805 | -10867.9673 | 18060.1564 | 8110.3876 | Mo | Cu | -5.0204 | 42876.4023 | 42396.5736 | 35249.3314 | Ti | Ni | -6.5810 | -44091.8875 | -45596.6355 | -45713.7833 |
| Cr | Al | -5.2906 | -11976.0028 | -9683.4768 | 6328.3893 | Mo | Fe | -8.8854 | 3061.7706 | 7843.8357 | 1932.9322 | Ti | Re | -11.1741 | -22882.0995 | -1814.4981 | -9289.1684 |
| Cr | Co | -7.6470 | 6172.5555 | 1680.9506 | -1617.9703 | Mo | Mn | -9.3112 | 2074.9220 | 5620.0504 | -4241.5090 | Ti | Ta | -10.6378 | -19396.3950 | 15427.3403 | 12624.8949 |
| Cr | Cr | -9.1155 | 38986.7181 | 30246.8730 | 29282.7317 | Mo | Mo | -10.4232 | 29604.1549 | 39458.6235 | 44890.2994 | Ti | Ti | -7.7045 | 5593.1269 | 3676.8749 | -2001.7552 |
| Cr | Cu | -4.9347 | 21945.3806 | 14699.3806 | 11883.8459 | Mo | Ni | -6.8227 | 4173.7964 | 8153.5535 | 3899.2390 | Ti | V | -8.4062 | 21835.3240 | 18974.4721 | 19089.6441 |
| Cr | Fe | -8.5634 | 4937.0530 | 9198.7580 | -6134.7353 | Mo | Re | -11.6578 | 2027.5087 | 10332.9327 | -3288.6350 | Ti | W | -11.2844 | -93265.2748 | 32153.0416 | 29885.8686 |
| Cr | Mn | -9.0167 | 1290.2095 | 7949.5550 | -3266.2724 | Mo | Ta | -11.3262 | -14243.3931 | 26131.9068 | 26553.1717 | V | Al | -5.1743 | -15153.4469 | -17307.2208 | -23627.5649 |
| Cr | Mo | -9.9624 | 44867.5994 | 51612.9450 | 46786.6623 | Mo | Ti | -8.4502 | 5227.3975 | 10147.4393 | 5627.3238 | V | Co | -7.7372 | -16922.0941 | -18196.6873 | -20886.8019 |
| Cr | Ni | -6.4440 | 11508.5378 | 11586.7506 | 8965.6027 | Mo | V | -9.1101 | 25498.7422 | 25389.7864 | 25987.0275 | V | Cr | -8.9731 | 38332.3809 | 29270.0548 | 27426.3302 |
| Cr | Re | -11.5619 | -17922.2124 | 13358.0476 | -8307.6080 | Mo | W | -8.4918 | 24775.6372 | 41243.8352 | 34871.0017 | V | Cu | -4.7347 | 26847.2286 | 27497.8995 | -8124.8655 |
| Cr | Ta | -10.8916 | -1502.5730 | 41202.2246 | 32493.1390 | Ni | Al | -4.4005 | -21166.3197 | -21366.5885 | -22108.3572 | V | Fe | -8.5231 | -5582.4412 | 68271.1655 | 65078.6967 |
| Cr | Ti | -7.9862 | 20801.6203 | 26860.3431 | 10325.9833 | Ni | Co | -6.7310 | -524.0824 | -3219.2033 | -9903.8520 | V | Mn | -8.9145 | -3251.2912 | -7444.0139 | -34465.8405 |
| Cr | V | -8.7636 | 29736.7011 | 35390.9098 | 30401.6193 | Ni | Cr | -8.3811 | 14766.6192 | 6984.4633 | -3911.3464 | V | Mo | -9.8870 | 37738.1780 | 37934.0445 | 44811.4813 |
| Cr | W | -11.4602 | -67845.4057 | 53176.5734 | 37449.0649 | Ni | Cu | -4.1808 | -390.3421 | -2773.6717 | -2341.6353 | V | Ni | -6.5564 | -13730.2979 | -18170.6913 | -34768.3514 |
| Cu | Al | -3.7793 | -6292.4695 | -11632.9250 | -25574.3510 | Ni | Fe | -7.4119 | 20953.1288 | 1091.6249 | -4987.0307 | V | Re | -11.3351 | -10434.8799 | 245.4416 | -11944.4376 |
| Cu | Co | -6.1438 | 11073.5714 | 8014.7609 | 5133.0460 | Ni | Mn | -8.1048 | -5805.0562 | -7337.0849 | -12237.6697 | V | Ta | -10.8398 | -10909.1368 | 22254.4614 | 22472.7676 |
| Cu | Cr | -7.7713 | 28550.3819 | 21705.1495 | 15672.1844 | Ni | Mo | -9.4739 | -3083.2505 | 9979.9873 | 7622.2608 | V | Ti | -7.9268 | 12133.6732 | 9332.7326 | 2076.1072 |
| Cu | Cu | -3.7330 | -2251.4534 | 5487.6698 | 6987.5478 | Ni | Ni | -5.5851 | -690.6879 | 100.0000 | 100.0000 | V | V | -8.6356 | 27692.0634 | 21133.7926 | 24032.9950 |
| Cu | Fe | -7.0424 | 11546.2393 | 8797.8108 | 6141.7728 | Ni | Re | -10.6128 | -21426.9335 | -495.4674 | -8787.6717 | V | W | -11.3687 | -73422.6970 | 40032.8178 | 37174.2412 |
| Cu | Mn | -7.4281 | 14430.8755 | 50304.8231 | 44437.2259 | Ni | Ta | -10.2110 | -30917.0142 | 2537.1853 | 299.2122 | W | Al | -5.9611 | -36863.8503 | 1826.7434 | -4187.6815 |
| Cu | Mo | -4.3389 | 44731.2853 | 55205.6712 | 55035.5854 | Ni | Ti | -7.2219 | -532.1540 | -7698.3663 | -3963.8291 | W | Co | -8.6225 | -48146.0150 | -13281.5785 | -18125.7273 |
| Cu | Ni | -5.0876 | 2242.7576 | 1142.9496 | 4064.1270 | Ni | V | -8.0502 | 3491.6474 | -2294.6338 | -6617.0036 | W | Cr | -9.8842 | 4617.7480 | 36161.0267 | 31718.8799 |
| Cu | Re | -9.8743 | 4765.8856 | 22253.8557 | 14387.6092 | Ni | W | -10.9543 | -11410.9150 | 13632.9699 | 6500.4751 | W | Cu | -5.3828 | 18507.0894 | 50060.6543 | 45735.2329 |
| Cu | Ta | -9.6564 | -22464.9644 | 12497.3028 | 11307.8977 | Re | Al | -5.8974 | -10810.7143 | -8391.0369 | -13821.3837 | W | Fe | -9.4184 | -37766.3396 | 4067.9133 | 1481.0424 |
| Cu | Ti | -6.7351 | 1378.8641 | -1330.9831 | -5347.6323 | Re | Co | -8.3355 | -544.6910 | 5681.8655 | 434.2725 | W | Mn | -9.8304 | -37421.1163 | 1714.7667 | -4569.8392 |
| Cu | V | -7.4548 | 15877.0771 | 11486.9418 | 7631.0000 | Re | Cr | -9.9072 | 22317.4780 | 21685.1473 | 12648.3953 | W | Mo | -8.4987 | 22588.8708 | 40919.7754 | 43639.0233 |
| Cu | W | -10.3920 | -10491.3407 | 14546.7629 | 11110.3277 | Re | Cu | -5.3185 | 44626.7035 | 41160.3233 | 10868.9189 | W | Ni | -7.0796 | -10018.6165 | 10546.6016 | 8636.5614 |
| Fe | Al | -4.9943 | -12489.1462 | -12481.7725 | -10986.6012 | Re | Fe | -9.2609 | -2655.6019 | 3296.9482 | -315.8322 | W | Re | -12.1563 | -35475.4148 | 8131.5809 | -3736.3235 |
| Fe | Co | -7.2264 | 17649.7478 | 4743.2270 | 1504.2328 | Re | Mn | -9.7861 | -13236.0023 | -5301.2733 | -12794.4505 | W | Ta | -11.8239 | -51660.6138 | 25786.8974 | 26654.9904 |
| Fe | Cr | -8.9643 | 24465.5688 | 17088.3791 | 9981.9412 | Re | Mo | -10.7406 | 29491.5960 | 98271.6303 | 98027.1324 | W | Ti | -8.9138 | -28901.5903 | 13171.9426 | 7603.6815 |
| Fe | Cu | -4.6548 | 19842.5021 | 31395.4154 | 33864.4311 | Re | Ni | -7.0831 | 9560.7619 | 16742.2119 | 22201.3584 | W | V | -9.6039 | -11540.5226 | 26223.3434 | 26745.0751 |
|  |  |  |  |  |  |  |  |  |  |  |  | W | W | -9.4974 | 16132.6257 | 36965.7016 | 31346.7792 |



**Fig. S1.**  The calculated and fitted temperature-dependent plot of the Gibbs free energy of Ni\_FCC (scattered data with a temperature step length of 10 K).

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**Fig. S2.** The Gibbs free energy of FCC\_L12 End-member (Al)1a (Ni)3c was calculated using QHA (solid line) and the fitted curve (red dash line) fitted by Eq (8). (scattered data with a temperature step length of 10 K).



**Fig. S3.** The calculated and fitted temperature-dependent Gibbs free energies of pure elements (scattered data with a temperature step length of 10 K).

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**Fig. S4.** The calculated temperature-dependent Gibbs free energies of FCC\_L12 end-members (A)1a(B)3c (scattered data with a temperature step length of 10 K).

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