Table : **List of possibly active surfaces for CO2 reduction. All the surfaces whose minimum CO adsorption energies were between -0.87 and -0.57 eV. MPID represents the Materials Project ID. Apparently duplicate entries for MPID/Miller index combinations are caused by different, non-identical cuts along a Miller plane, which yields multiple surfaces for a single Miller index. All energies reported here were calculated by DFT, not with machine learning.**

|  |  |  |  |
| --- | --- | --- | --- |
| Formula | Miller Indices | ΔECO | MPID |
| Ag3Pd | [2 0 1] | -0.84 | mp-985296 |
| Al2Cu | [1 1 0] | -0.66 | mp-985806 |
| Al2Cu | [1 1 1] | -0.75 | mp-985806 |
| Al2Cu | [1 1 1] | -0.73 | mp-985806 |
| Al2Cu | [2 1 0] | -0.75 | mp-985806 |
| Al2Cu | [2 1 0] | -0.68 | mp-985806 |
| Al2Cu | [2 2 1] | -0.73 | mp-985806 |
| Al2Cu6 | [0 0 1] | -0.79 | mp-12802 |
| Al2Cu6 | [0 0 1] | -0.64 | mp-12802 |
| Al2Cu6 | [1 1 0] | -0.8 | mp-12802 |
| Al2Cu6 | [1 1 2] | -0.84 | mp-12802 |
| Al2Cu6 | [1 2 0] | -0.65 | mp-12802 |
| Al2Cu6 | [1 2 1] | -0.69 | mp-12802 |
| Al2Cu6 | [1 2 2] | -0.78 | mp-12802 |
| Al2Cu6 | [2 1 0] | -0.7 | mp-12802 |
| Al2Cu6 | [2 2 1] | -0.76 | mp-12802 |
| Al3Cu2 | [1 1 1] | -0.83 | mp-10886 |
| Al3Cu2 | [1 1 1] | -0.82 | mp-10886 |
| Al3Cu2 | [2 0 1] | -0.82 | mp-10886 |
| Al5Cu5 | [1 1 -2] | -0.83 | mp-2500 |
| Al6Cu2 | [1 0 1] | -0.58 | mp-985825 |
| Al6Cu2 | [2 1 0] | -0.83 | mp-985825 |
| AlCu | [1 1 1] | -0.8 | mp-1022721 |
| AlCu3 | [1 1 0] | -0.76 | mp-1008555 |
| AlCu3 | [1 1 0] | -0.72 | mp-1008555 |
| AlCu3 | [1 1 1] | -0.84 | mp-12777 |
| AlCu3 | [2 1 0] | -0.78 | mp-1008555 |
| AlCu3 | [2 1 0] | -0.75 | mp-1008555 |
| Al2N2 | [2 1 2] | -0.66 | mp-661 |
| Al2Pd | [2 2 1] | -0.85 | mp-16522 |
| Al6Pd10 | [1 0 0] | -0.78 | mp-16523 |
| AlPd | [1 0 0] | -0.85 | mp-829 |
| Al2Pt | [1 0 0] | -0.72 | mp-1502 |
| Al2Ti2 | [0 0 1] | -0.6 | mp-1953 |
| Al4Ti2 | [0 0 1] | -0.82 | mp-11809 |
| Al12W | [1 0 0] | -0.77 | mp-11227 |
| AsGa | [1 0 0] | -0.81 | mp-2534 |
| AsGa | [2 1 1] | -0.76 | mp-2534 |
| As4Si3 | [1 1 1] | -0.87 | mp-570744 |
| As6Si6 | [2 2 -1] | -0.67 | mp-1863 |
| As4Zn4Cu4 | [1 0 1] | -0.66 | mp-676828 |
| As4Zn4Cu4 | [1 2 1] | -0.75 | mp-676828 |
| As4Zn4Cu4 | [2 1 0] | -0.75 | mp-676828 |
| As4Zn4Cu4 | [2 1 2] | -0.79 | mp-676828 |
| Au2Al | [0 0 1] | -0.73 | mp-1018179 |
| Au2Al | [1 0 2] | -0.74 | mp-1018179 |
| Au4Al4 | [0 0 1] | -0.62 | mp-1399 |
| Au2AlCu | [1 1 1] | -0.73 | mp-867306 |
| Au2AlCu | [2 1 0] | -0.79 | mp-867306 |
| Au2Cu2 | [0 0 1] | -0.67 | mp-522 |
| Au2Cu2 | [1 0 0] | -0.69 | mp-522 |
| Au2Cu2 | [2 1 0] | -0.84 | mp-522 |
| Au3Cu | [2 1 0] | -0.76 | mp-2103 |
| Au3Cu | [2 1 0] | -0.61 | mp-2103 |
| Au3Cu | [2 1 1] | -0.64 | mp-2103 |
| Au3Cu | [2 2 1] | -0.71 | mp-2103 |
| AuCu3 | [1 1 0] | -0.68 | mp-2258 |
| AuCu3 | [1 1 0] | -0.63 | mp-2258 |
| AuCu3 | [2 1 0] | -0.8 | mp-2258 |
| AuCu3 | [2 1 0] | -0.79 | mp-2258 |
| AuCu3 | [2 1 1] | -0.75 | mp-2258 |
| AuGa2 | [1 0 0] | -0.57 | mp-2776 |
| AuPd2In | [2 2 1] | -0.79 | mp-863724 |
| Au5Sn | [1 1 0] | -0.64 | mp-30418 |
| Au4Ti | [1 1 0] | -0.58 | mp-12635 |
| Co8Al20 | [0 0 1] | -0.69 | mp-196 |
| Cu | [1 1 0] | -0.63 | mp-30 |
| Cu | [2 1 0] | -0.78 | mp-30 |
| Cu | [2 1 1] | -0.69 | mp-30 |
| CuAlPt2 | [1 1 0] | -0.77 | mp-12550 |
| Cu28In12 | [0 0 1] | -0.84 | mp-21985 |
| Fe2Al12 | [1 1 0] | -0.69 | mp-570001 |
| FeAl | [1 0 0] | -0.6 | mp-2658 |
| Ga2Cu | [0 0 1] | -0.78 | mp-11359 |
| Ga2Cu | [1 0 0] | -0.64 | mp-11359 |
| Ga2Cu | [1 0 1] | -0.67 | mp-11359 |
| Ga2Cu | [1 1 1] | -0.66 | mp-11359 |
| Ga2Cu | [1 1 2] | -0.74 | mp-11359 |
| Ga2Cu | [2 0 1] | -0.72 | mp-11359 |
| Ga2Cu | [2 1 0] | -0.82 | mp-11359 |
| Ga2Cu6 | [1 0 0] | -0.79 | mp-865798 |
| Ga2Cu6 | [1 0 0] | -0.69 | mp-865798 |
| Ga2Cu6 | [1 0 1] | -0.75 | mp-865798 |
| Ga2Cu6 | [1 1 0] | -0.8 | mp-865798 |
| Ga2Cu6 | [1 1 1] | -0.72 | mp-865798 |
| Ga2Cu6 | [2 2 1] | -0.84 | mp-865798 |
| Ga10Pd2 | [1 1 2] | -0.66 | mp-30660 |
| Ga6Pd10 | [1 0 0] | -0.79 | mp-2408 |
| Ga2Pt | [1 0 0] | -0.64 | mp-22095 |
| Ga2Pt | [1 1 0] | -0.65 | mp-22095 |
| Ga2Pt | [2 1 0] | -0.7 | mp-22095 |
| Ga3Pt2 | [1 1 0] | -0.65 | mp-21400 |
| Ga3Pt2 | [2 1 1] | -0.68 | mp-21400 |
| Ga3Pt2 | [2 2 1] | -0.81 | mp-21400 |
| GaPt2Cu | [1 1 0] | -0.74 | mp-644280 |
| Ge2 | [2 1 1] | -0.75 | mp-32 |
| Ge4Co4Cu2 | [1 0 0] | -0.71 | mp-19955 |
| Ge2Cu6 | [1 0 2] | -0.71 | mp-19724 |
| Ge2Cu6 | [1 2 1] | -0.75 | mp-19724 |
| Ge2Cu6 | [2 1 0] | -0.72 | mp-19724 |
| Ge4Fe4Cu2 | [1 0 0] | -0.7 | mp-21141 |
| H6Al2 | [2 1 1] | -0.74 | mp-23933 |
| H2Si2 | [1 0 0] | -0.77 | mp-29803 |
| H2Si2 | [2 0 1] | -0.85 | mp-29803 |
| H2Ti | [0 0 1] | -0.68 | mp-24726 |
| H2Ti | [1 0 0] | -0.64 | mp-24161 |
| H2Ti | [1 1 0] | -0.63 | mp-24726 |
| Ir4In12 | [0 2 1] | -0.86 | mp-636498 |
| IrRhGa2 | [1 0 0] | -0.81 | mp-865743 |
| Mn2Al2 | [0 0 1] | -0.74 | mp-771 |
| Mn3GaN | [1 0 0] | -0.85 | mp-627439 |
| N4 | [1 1 0] | -0.84 | mp-999498 |
| NIn | [1 0 0] | -0.76 | mp-20411 |
| N2V2 | [1 1 1] | -0.74 | mp-1017532 |
| N2V2 | [2 1 0] | -0.77 | mp-1017532 |
| Ni4Al12 | [0 0 1] | -0.64 | mp-622209 |
| NiAl | [1 0 0] | -0.69 | mp-1487 |
| NiFeAl2 | [1 0 0] | -0.73 | mp-867330 |
| NiGa | [1 1 1] | -0.75 | mp-1941 |
| Ni4Si4 | [0 1 0] | -0.7 | mp-351 |
| NiZnCu2 | [1 0 0] | -0.68 | mp-30593 |
| NiZnCu2 | [1 1 0] | -0.87 | mp-30593 |
| OsAl | [1 0 0] | -0.73 | mp-875 |
| Pd4Cu16 | [0 0 1] | -0.71 | mp-30594 |
| Pd4Cu16 | [2 1 0] | -0.82 | mp-30594 |
| PdCu | [1 0 0] | -0.66 | mp-1018029 |
| PdCu3 | [1 0 0] | -0.66 | mp-580357 |
| PdCu3 | [1 1 0] | -0.76 | mp-580357 |
| PdCu3 | [1 1 1] | -0.82 | mp-580357 |
| PdCu3 | [2 2 1] | -0.84 | mp-580357 |
| Pd2CuIn | [1 0 0] | -0.79 | mp-867308 |
| PtCu | [0 0 1] | -0.72 | mp-644311 |
| PtCu3 | [1 0 0] | -0.69 | mp-12086 |
| PtCu3 | [1 1 0] | -0.79 | mp-12086 |
| PtCu3 | [2 2 1] | -0.76 | mp-12086 |
| PtIn2 | [2 1 0] | -0.74 | mp-22682 |
| Re2Al12 | [0 0 1] | -0.66 | mp-16528 |
| Re2Al12 | [1 1 0] | -0.7 | mp-16528 |
| ReAl12 | [1 0 0] | -0.8 | mp-1648 |
| RuCoGa2 | [1 0 0] | -0.69 | mp-865779 |
| RuIrGa2 | [1 0 0] | -0.65 | mp-866041 |
| Sb2Al2 | [1 0 2] | -0.82 | mp-1018100 |
| SbAl | [1 1 1] | -0.82 | mp-2624 |
| SbAl | [2 1 1] | -0.8 | mp-2624 |
| SbCuNi2 | [1 0 0] | -0.66 | mp-30069 |
| Sb2Ga2 | [2 0 1] | -0.76 | mp-1018059 |
| SbGa | [1 1 1] | -0.57 | mp-1156 |
| Sb2Pd2 | [1 1 1] | -0.57 | mp-1769 |
| Sb2Pd2 | [2 2 1] | -0.58 | mp-1769 |
| Sb8Pd4 | [2 1 0] | -0.71 | mp-1356 |
| Sb2Pt2 | [1 0 1] | -0.61 | mp-2845 |
| Sb2Pt2 | [1 1 0] | -0.67 | mp-2845 |
| Sb2Pt2 | [2 -1 2] | -0.61 | mp-2845 |
| Sb2Pt2 | [2 1 0] | -0.68 | mp-2845 |
| Si2Cu6 | [1 0 0] | -0.6 | mp-867317 |
| Si2Cu6 | [1 0 2] | -0.73 | mp-867317 |
| Si2Cu6 | [1 0 2] | -0.73 | mp-867317 |
| Si2Cu6 | [1 1 0] | -0.78 | mp-867317 |
| Si2Cu6 | [1 1 1] | -0.79 | mp-867317 |
| Si2Cu6 | [2 0 1] | -0.83 | mp-867317 |
| Si2Cu6 | [2 1 1] | -0.71 | mp-867317 |
| SiCu3 | [0 0 1] | -0.65 | mp-972828 |
| SiCu3 | [1 0 0] | -0.69 | mp-972828 |
| SiCu3 | [2 0 1] | -0.82 | mp-972828 |
| SiCu3 | [2 1 0] | -0.77 | mp-972828 |
| SiCu3 | [2 1 1] | -0.81 | mp-972828 |
| SiCu3 | [2 1 1] | -0.79 | mp-972828 |
| Si16Fe8 | [0 1 0] | -0.86 | mp-1714 |
| Si4Pd4 | [0 1 1] | -0.83 | mp-389 |
| Si4Pd4 | [1 0 0] | -0.63 | mp-389 |
| Si4Pt4 | [1 0 1] | -0.8 | mp-696 |
| Si4Pt4 | [1 2 0] | -0.67 | mp-696 |
| Si4Rh4 | [0 1 0] | -0.83 | mp-818 |
| Sn10Cu12 | [0 1 0] | -0.64 | mp-1233 |
| Sn10Cu12 | [1 0 0] | -0.68 | mp-1233 |
| Sn10Cu12 | [1 1 -2] | -0.7 | mp-1233 |
| Sn16Cu20 | [0 0 1] | -0.65 | mp-845 |
| Sn16Cu20 | [1 0 0] | -0.63 | mp-845 |
| Sn16Cu20 | [1 0 0] | -0.61 | mp-845 |
| Sn2Cu2 | [2 1 1] | -0.61 | mp-10598 |
| Sn12Pd4 | [1 1 2] | -0.76 | mp-1371 |
| Sn12Pd4 | [1 2 1] | -0.77 | mp-1371 |
| Sn12Pd4 | [2 0 1] | -0.74 | mp-1371 |
| Sn16Pd8 | [1 1 0] | -0.66 | mp-1573 |
| Sn4Pd4 | [1 0 0] | -0.58 | mp-2369 |
| Sn2Pt | [1 1 0] | -0.69 | mp-19962 |
| Sn2Pt2 | [1 0 1] | -0.75 | mp-19856 |
| Sn2Pt2 | [2 -1 2] | -0.74 | mp-19856 |
| Sn2Pt2 | [2 1 0] | -0.85 | mp-19856 |
| Zn4Au2Cu2 | [0 1 2] | -0.62 | mp-12759 |
| Zn4Au2Cu2 | [1 1 1] | -0.68 | mp-12759 |
| Zn4Au2Cu2 | [1 2 1] | -0.63 | mp-12759 |
| Zn4Au2Cu2 | [1 2 2] | -0.79 | mp-12759 |
| ZnAu2Cu | [1 0 0] | -0.78 | mp-864623 |
| ZnAu2Cu | [2 1 0] | -0.72 | mp-864623 |
| Zn16Cu10 | [1 1 0] | -0.82 | mp-1368 |
| ZnCu | [1 0 0] | -0.61 | mp-987 |
| ZnCu | [2 1 0] | -0.79 | mp-987 |
| Zn2Pd2 | [2 0 1] | -0.58 | mp-1652 |

Table : **List of possibly efficient surfaces for H2 evolution. All the surfaces whose minimum H adsorption energies were between -0.47 and -0.17 eV. MPID represents the Materials Project ID. Apparently duplicate entries for MPID/Miller index combinations are caused by different, non-identical cuts along a Miller plane, which yields multiple surfaces for a single Miller index. All energies reported here were calculated by DFT, not with machine learning.**

|  |  |  |  |
| --- | --- | --- | --- |
| Formula | Miller Indices | ΔEH | MPID |
| Ag3Pd | [1 0 0] | -0.24 | mp-985296 |
| Al2Cu | [1 1 1] | -0.45 | mp-985806 |
| Al2Cu | [1 1 1] | -0.21 | mp-985806 |
| Al2Cu | [2 1 0] | -0.34 | mp-985806 |
| Al2Cu | [2 1 0] | -0.28 | mp-985806 |
| Al2Cu | [2 1 1] | -0.37 | mp-985806 |
| Al2Cu6 | [1 1 0] | -0.18 | mp-12802 |
| Al2Cu6 | [1 1 1] | -0.21 | mp-12802 |
| Al2Cu6 | [1 2 2] | -0.21 | mp-12802 |
| Al3Cu2 | [1 1 1] | -0.2 | mp-10886 |
| Al4Cu2 | [1 0 1] | -0.22 | mp-998 |
| Al4Cu2 | [1 1 2] | -0.23 | mp-998 |
| Al5Cu5 | [1 1 -1] | -0.17 | mp-2500 |
| Al5Cu5 | [1 1 -2] | -0.25 | mp-2500 |
| Al6Cu2 | [1 1 1] | -0.22 | mp-985825 |
| Al6Cu2 | [1 1 2] | -0.2 | mp-985825 |
| AlCu3 | [1 1 1] | -0.3 | mp-12777 |
| Al2Pd | [2 1 0] | -0.37 | mp-16522 |
| Al4Pd4 | [1 0 0] | -0.22 | mp-7189 |
| Al4Pd8 | [0 0 1] | -0.24 | mp-2824 |
| Al2Pt | [2 2 1] | -0.37 | mp-1502 |
| Al3Pt2 | [2 1 1] | -0.46 | mp-10905 |
| Al4Pt12 | [0 0 1] | -0.29 | mp-607111 |
| Al4Pt12 | [1 0 1] | -0.4 | mp-607111 |
| Al4Pt4 | [1 0 0] | -0.42 | mp-10904 |
| Al4Pt4 | [2 1 1] | -0.38 | mp-10904 |
| Al4Pt4 | [2 1 1] | -0.34 | mp-10904 |
| Al4Pt8 | [0 0 1] | -0.42 | mp-16526 |
| Al4Pt8 | [1 0 0] | -0.37 | mp-16526 |
| Al6Pt10 | [1 0 0] | -0.34 | mp-1501 |
| AlPt3 | [1 0 0] | -0.38 | mp-188 |
| AlPt3 | [1 1 1] | -0.45 | mp-188 |
| Al3V | [1 1 0] | -0.46 | mp-2554 |
| Al3V | [1 1 1] | -0.35 | mp-2554 |
| Al3V | [1 1 2] | -0.33 | mp-2554 |
| Al12W | [1 1 1] | -0.47 | mp-11227 |
| As2 | [1 1 1] | -0.21 | mp-11 |
| As2 | [2 1 0] | -0.47 | mp-11 |
| As2 | [2 2 1] | -0.23 | mp-11 |
| As4Co4 | [1 0 0] | -0.43 | mp-15679 |
| As4Co4 | [1 1 0] | -0.45 | mp-583 |
| As2Ga2 | [2 2 1] | -0.19 | mp-8883 |
| AsGa | [2 1 0] | -0.21 | mp-2534 |
| AsIn | [2 1 0] | -0.44 | mp-20305 |
| As4Os2 | [1 1 1] | -0.37 | mp-2455 |
| AsPd5In | [2 1 0] | -0.23 | mp-1025293 |
| AsPd5In | [2 1 2] | -0.46 | mp-1025293 |
| As4Rh4 | [0 0 1] | -0.46 | mp-22079 |
| As4Rh4 | [0 0 1] | -0.19 | mp-22079 |
| As4Rh4 | [1 0 2] | -0.25 | mp-22079 |
| As4Rh4 | [2 2 1] | -0.45 | mp-22079 |
| As4Rh4 | [2 2 1] | -0.33 | mp-22079 |
| As8Rh4 | [1 0 -1] | -0.45 | mp-15954 |
| As2Rh10Ga4 | [1 0 0] | -0.46 | mp-18561 |
| As6Si6 | [1 1 0] | -0.2 | mp-1863 |
| AsSn | [1 1 1] | -0.23 | mp-2182 |
| As6Ti8 | [1 1 0] | -0.33 | mp-567082 |
| As4Zn4Cu4 | [1 1 1] | -0.36 | mp-676828 |
| As4Zn4Cu4 | [1 1 1] | -0.24 | mp-676828 |
| As4Zn4Cu4 | [1 2 1] | -0.31 | mp-676828 |
| As4Zn4Cu4 | [2 1 0] | -0.3 | mp-676828 |
| AsZnPt5 | [0 0 1] | -0.4 | mp-1025356 |
| AsZnPt5 | [1 1 1] | -0.44 | mp-1025356 |
| Au4Al4 | [0 0 1] | -0.29 | mp-1399 |
| Au4Al4 | [0 0 1] | -0.21 | mp-1399 |
| Au4Al4 | [2 2 1] | -0.3 | mp-1399 |
| AuAl2 | [1 1 1] | -0.46 | mp-2647 |
| AuAl2 | [2 1 0] | -0.36 | mp-2647 |
| AuAl2 | [2 2 1] | -0.37 | mp-2647 |
| Au2AlCu | [2 1 0] | -0.28 | mp-867306 |
| Au3Pd | [2 1 1] | -0.19 | mp-973834 |
| AuPd3 | [1 0 0] | -0.3 | mp-999298 |
| AuPd3 | [1 0 0] | -0.18 | mp-999298 |
| AuPd3 | [2 1 1] | -0.4 | mp-999298 |
| AuPd3 | [2 1 1] | -0.36 | mp-999298 |
| AuPd3 | [2 2 1] | -0.29 | mp-999298 |
| AuPdCu2 | [2 1 0] | -0.19 | mp-862256 |
| Co4Al18 | [0 0 1] | -0.41 | mp-16488 |
| CoFeAl2 | [2 1 0] | -0.45 | mp-862691 |
| Co4Ga12 | [1 0 1] | -0.21 | mp-20559 |
| Co4Ga12 | [1 1 0] | -0.18 | mp-20559 |
| Co4In12 | [1 0 0] | -0.33 | mp-22236 |
| Co4In12 | [2 1 0] | -0.31 | mp-22236 |
| Co4N2 | [1 0 1] | -0.41 | mp-22631 |
| Co2Pt2 | [1 0 1] | -0.4 | mp-949 |
| CoPt3 | [1 0 0] | -0.36 | mp-922 |
| CoPt3 | [2 1 0] | -0.36 | mp-922 |
| CoPt3 | [2 2 1] | -0.37 | mp-922 |
| Co2Sn4 | [1 1 1] | -0.24 | mp-20155 |
| Co2Sn4 | [1 1 1] | -0.18 | mp-20155 |
| Co2Sn4 | [2 1 1] | -0.2 | mp-20155 |
| Co3Sn3 | [2 1 1] | -0.4 | mp-20536 |
| CrCoPt2 | [1 1 1] | -0.35 | mp-570863 |
| CrCoPt2 | [1 1 2] | -0.36 | mp-570863 |
| CrCoPt2 | [2 1 0] | -0.45 | mp-570863 |
| CrCoPt2 | [2 1 0] | -0.39 | mp-570863 |
| CuAlPt2 | [0 0 1] | -0.4 | mp-12550 |
| CuAlPt2 | [1 0 0] | -0.27 | mp-12550 |
| CuAlPt2 | [1 1 1] | -0.33 | mp-12550 |
| CuAlPt2 | [1 1 2] | -0.29 | mp-12550 |
| CuAlPt2 | [2 1 0] | -0.43 | mp-12550 |
| CuAlPt2 | [2 1 2] | -0.44 | mp-12550 |
| Cu28In12 | [0 1 0] | -0.29 | mp-21985 |
| Fe2Al12 | [0 0 1] | -0.3 | mp-570001 |
| Fe2Al6 | [1 0 0] | -0.43 | mp-984873 |
| Fe2Al6 | [1 1 0] | -0.24 | mp-984873 |
| Fe2Al6 | [2 1 1] | -0.46 | mp-984873 |
| Fe4Ga12 | [1 0 1] | -0.33 | mp-636368 |
| Fe4Ga12 | [1 1 0] | -0.25 | mp-636368 |
| Fe2Pd2 | [1 0 1] | -0.44 | mp-2831 |
| Fe2Pd2 | [1 1 0] | -0.3 | mp-2831 |
| Fe2Pd2 | [2 1 2] | -0.35 | mp-2831 |
| Fe2Pd2 | [2 1 2] | -0.33 | mp-2831 |
| FePd3 | [1 0 0] | -0.3 | mp-21845 |
| FePt | [1 0 0] | -0.4 | mp-2260 |
| FePt | [1 1 1] | -0.41 | mp-2260 |
| FePt | [2 0 1] | -0.41 | mp-2260 |
| FePt | [2 1 1] | -0.47 | mp-2260 |
| Fe2WAl | [1 0 0] | -0.44 | mp-862288 |
| Fe2WAl | [2 1 0] | -0.44 | mp-862288 |
| Ga2N2 | [1 0 1] | -0.37 | mp-804 |
| Ga10Pd2 | [1 1 0] | -0.27 | mp-30660 |
| Ga3Pd7 | [0 0 1] | -0.27 | mp-31467 |
| Ga3Pd7 | [1 0 0] | -0.38 | mp-31467 |
| Ga3Pd7 | [1 0 0] | -0.35 | mp-31467 |
| Ga3Pd7 | [1 1 -1] | -0.31 | mp-31467 |
| Ga4Pd8 | [0 0 1] | -0.27 | mp-1869 |
| Ga4Pd8 | [0 1 0] | -0.24 | mp-1869 |
| Ga4Pd8 | [1 0 1] | -0.24 | mp-1869 |
| Ga4Pd8 | [1 0 1] | -0.23 | mp-1869 |
| Ga4Pd8 | [1 1 0] | -0.34 | mp-1869 |
| Ga4Pd8 | [1 1 0] | -0.31 | mp-1869 |
| Ga4Pd8 | [2 1 0] | -0.32 | mp-1869 |
| Ga6Pd10 | [0 0 1] | -0.34 | mp-2408 |
| Ga2Pd2Ti2 | [1 0 0] | -0.26 | mp-1025045 |
| Ga2Pt6 | [0 0 1] | -0.27 | mp-862621 |
| Ga2Pt6 | [0 0 1] | -0.19 | mp-862621 |
| Ga2Pt6 | [1 0 1] | -0.42 | mp-862621 |
| Ga2Pt6 | [1 0 2] | -0.42 | mp-862621 |
| Ga3Pt5 | [0 0 1] | -0.43 | mp-30663 |
| Ga3Pt5 | [0 1 0] | -0.39 | mp-30663 |
| Ga3Pt5 | [0 1 1] | -0.43 | mp-30663 |
| Ga3Pt5 | [0 1 1] | -0.43 | mp-30663 |
| Ga3Pt5 | [1 1 2] | -0.43 | mp-30663 |
| Ga4Pt12 | [0 0 1] | -0.32 | mp-623066 |
| Ga4Pt12 | [1 0 2] | -0.43 | mp-623066 |
| Ga8Pt16 | [1 0 0] | -0.45 | mp-2223 |
| GaPt3 | [1 0 0] | -0.46 | mp-11407 |
| GaPt3 | [1 1 0] | -0.33 | mp-11407 |
| GaPt3 | [2 1 1] | -0.42 | mp-11407 |
| GaPt2Cu | [1 0 0] | -0.44 | mp-644280 |
| GaPt2Cu | [1 0 2] | -0.42 | mp-644280 |
| GaPt2Cu | [1 1 0] | -0.45 | mp-644280 |
| GaPt2Cu | [1 1 0] | -0.35 | mp-862791 |
| GaPt2Cu | [1 1 1] | -0.39 | mp-862791 |
| GaPt2Cu | [1 1 2] | -0.35 | mp-644280 |
| GaPt2Cu | [2 0 1] | -0.46 | mp-644280 |
| GaPt2Cu | [2 1 0] | -0.41 | mp-644280 |
| GaPt2Cu | [2 1 1] | -0.28 | mp-644280 |
| GaPt2Cu | [2 1 2] | -0.37 | mp-644280 |
| GaPt2Cu | [2 2 1] | -0.44 | mp-644280 |
| Ge4Co4Cu2 | [1 0 0] | -0.22 | mp-19955 |
| Ge2Cu6 | [1 1 2] | -0.21 | mp-19724 |
| Ge2Cu6 | [1 2 1] | -0.18 | mp-19724 |
| Ge2Mn2Ga2 | [2 0 1] | -0.47 | mp-1018802 |
| Ge2Mo | [1 1 2] | -0.35 | mp-10201 |
| GePtTi | [2 1 0] | -0.45 | mp-1008680 |
| Ge4Rh4 | [0 0 1] | -0.44 | mp-22239 |
| Ge4Rh4 | [0 2 1] | -0.38 | mp-22239 |
| Ge4Rh4 | [1 0 0] | -0.28 | mp-20866 |
| Ir | [1 1 1] | -0.37 | mp-101 |
| Ir2Al6 | [0 0 1] | -0.44 | mp-2294 |
| Ir2Al6 | [0 0 1] | -0.41 | mp-2294 |
| Ir2Al6 | [1 0 0] | -0.46 | mp-2294 |
| Ir2Al6 | [1 0 0] | -0.26 | mp-2294 |
| Ir2Al6 | [2 -1 2] | -0.33 | mp-2294 |
| IrFeAl2 | [1 1 0] | -0.45 | mp-866031 |
| Ir4Ga18 | [1 2 0] | -0.31 | mp-31311 |
| Ir6Ga12 | [0 0 1] | -0.43 | mp-31253 |
| Ir6Ga12 | [1 1 0] | -0.37 | mp-31253 |
| IrGa | [1 1 1] | -0.46 | mp-11388 |
| Ir4In8 | [0 1 0] | -0.38 | mp-22812 |
| IrRhAl2 | [1 1 1] | -0.33 | mp-862694 |
| Ir6Sn14 | [1 0 0] | -0.21 | mp-22040 |
| IrSn2 | [1 0 0] | -0.31 | mp-2083 |
| IrSn2 | [2 1 1] | -0.22 | mp-2083 |
| Ir6V2 | [1 1 0] | -0.39 | mp-865496 |
| MnRh2In | [2 1 0] | -0.47 | mp-864968 |
| Mn2RhPt | [2 1 0] | -0.39 | mp-865032 |
| Mn2RhPt | [2 1 0] | -0.33 | mp-865032 |
| MnRhTi2 | [1 0 0] | -0.39 | mp-866218 |
| MoN | [2 2 1] | -0.38 | mp-13036 |
| MoZn7 | [1 1 1] | -0.4 | mp-644500 |
| N2V2 | [2 1 0] | -0.18 | mp-1017532 |
| Ni | [1 1 0] | -0.41 | mp-23 |
| Ni2Al3 | [1 1 1] | -0.38 | mp-1057 |
| Ni2Al3 | [2 -1 2] | -0.45 | mp-1057 |
| Ni2Al3 | [2 1 0] | -0.3 | mp-1057 |
| Ni2Al3 | [2 2 1] | -0.32 | mp-1057 |
| Ni4Al12 | [0 0 1] | -0.35 | mp-622209 |
| Ni4Al12 | [0 1 0] | -0.4 | mp-622209 |
| Ni5Al3 | [0 0 1] | -0.41 | mp-16514 |
| Ni5Al3 | [0 2 1] | -0.31 | mp-16514 |
| Ni5Al3 | [1 1 2] | -0.46 | mp-16514 |
| Ni5Al3 | [1 1 2] | -0.45 | mp-16514 |
| Ni5Al3 | [2 0 1] | -0.32 | mp-16514 |
| NiAl | [1 0 0] | -0.36 | mp-1487 |
| NiAl | [1 1 1] | -0.23 | mp-1487 |
| NiAl | [2 1 0] | -0.43 | mp-1487 |
| Ni2AuSn4 | [1 0 1] | -0.23 | mp-568925 |
| NiCo2Ga | [1 0 0] | -0.32 | mp-20551 |
| NiCo2Ga | [2 1 1] | -0.41 | mp-1018060 |
| Ni2Fe2 | [1 0 0] | -0.41 | mp-2213 |
| Ni2Fe2 | [2 1 0] | -0.42 | mp-2213 |
| Ni2Fe2 | [2 1 2] | -0.41 | mp-2213 |
| Ni3Fe | [1 0 0] | -0.4 | mp-1007855 |
| Ni3Fe | [1 1 0] | -0.42 | mp-1418 |
| NiFeAl2 | [2 1 0] | -0.4 | mp-867330 |
| NiFePt2 | [0 0 1] | -0.39 | mp-13463 |
| NiFePt2 | [0 0 1] | -0.31 | mp-13463 |
| NiFePt2 | [1 0 0] | -0.39 | mp-13463 |
| NiFePt2 | [1 0 0] | -0.37 | mp-13463 |
| NiFePt2 | [1 1 1] | -0.38 | mp-13463 |
| NiFePt2 | [2 1 1] | -0.45 | mp-13463 |
| Ni13Ga9 | [1 0 0] | -0.42 | mp-21589 |
| Ni2Ga3 | [2 -1 2] | -0.43 | mp-11397 |
| Ni2Ga3 | [2 -1 2] | -0.43 | mp-11397 |
| Ni4Ga2 | [1 1 1] | -0.39 | mp-570904 |
| Ni5Ga3 | [0 0 1] | -0.44 | mp-11398 |
| Ni4Ge4 | [1 0 2] | -0.37 | mp-1099 |
| Ni2In3 | [1 1 1] | -0.22 | mp-21385 |
| Ni6Mo2 | [0 1 0] | -0.46 | mp-11506 |
| Ni2Pt2 | [0 0 1] | -0.36 | mp-945 |
| Ni2Pt2 | [1 0 1] | -0.39 | mp-945 |
| Ni2Pt2 | [2 1 0] | -0.47 | mp-945 |
| Ni2Pt2 | [2 1 0] | -0.39 | mp-945 |
| Ni2Pt2 | [2 2 1] | -0.45 | mp-945 |
| Ni2Pt2 | [2 2 1] | -0.42 | mp-945 |
| Ni3Pt | [1 0 0] | -0.43 | mp-12798 |
| Ni3Pt | [1 0 0] | -0.33 | mp-12798 |
| NiRh2Ga | [1 1 1] | -0.44 | mp-866037 |
| NiRh2Ga | [2 1 0] | -0.43 | mp-866037 |
| NiRh2Sn | [1 1 1] | -0.4 | mp-11519 |
| Ni2Si2 | [0 0 1] | -0.31 | mp-999192 |
| Ni2Si2 | [1 2 1] | -0.38 | mp-999192 |
| Ni2Si2 | [1 2 2] | -0.36 | mp-999192 |
| Ni2Si2 | [2 1 2] | -0.36 | mp-999192 |
| Ni4Si4 | [1 0 2] | -0.39 | mp-351 |
| Ni8Si4 | [1 1 1] | -0.45 | mp-1118 |
| Ni3Sn4 | [1 1 -2] | -0.28 | mp-20174 |
| Ni6Sn2 | [1 0 0] | -0.17 | mp-20112 |
| Ni3SnN | [2 1 1] | -0.4 | mp-1017632 |
| Ni4W | [0 0 1] | -0.4 | mp-30811 |
| OsAl | [1 0 0] | -0.29 | mp-875 |
| Os4Ga12 | [0 0 1] | -0.29 | mp-570844 |
| OsV3 | [1 1 1] | -0.41 | mp-866121 |
| PbMnRh2 | [2 1 0] | -0.36 | mp-4652 |
| Pb4Pt2 | [1 0 1] | -0.27 | mp-21318 |
| Pb10Rh8 | [0 1 0] | -0.18 | mp-569678 |
| Pd | [1 1 0] | -0.41 | mp-2 |
| Pd | [1 1 1] | -0.45 | mp-2 |
| Pd4Cu16 | [1 0 0] | -0.19 | mp-30594 |
| PdCu3 | [1 1 1] | -0.22 | mp-580357 |
| PdCu3 | [2 2 1] | -0.2 | mp-580357 |
| Pd2CuIn | [1 0 0] | -0.21 | mp-867308 |
| Pd2CuIn | [1 1 0] | -0.24 | mp-867308 |
| Pd2CuIn | [2 1 0] | -0.2 | mp-867308 |
| Pd3In | [1 0 2] | -0.36 | mp-510436 |
| Pd3In | [1 1 1] | -0.42 | mp-510436 |
| Pd3In | [2 0 1] | -0.39 | mp-510436 |
| Pd3In | [2 0 1] | -0.36 | mp-510436 |
| Pd3In | [2 1 0] | -0.39 | mp-31337 |
| Pd3In | [2 1 0] | -0.36 | mp-31337 |
| Pd3In | [2 1 2] | -0.46 | mp-510436 |
| Pd3In | [2 1 2] | -0.4 | mp-510436 |
| Pd8In4 | [1 0 2] | -0.36 | mp-22646 |
| Pd8In4 | [1 1 0] | -0.38 | mp-22646 |
| Pd8In4 | [2 1 0] | -0.23 | mp-22646 |
| Pd2Ti | [1 1 0] | -0.42 | mp-1018121 |
| Pd2Ti | [1 1 2] | -0.37 | mp-1018121 |
| Pd2Ti | [2 1 2] | -0.47 | mp-1018121 |
| Pd2V | [1 0 1] | -0.26 | mp-11549 |
| Pd2V | [1 1 0] | -0.44 | mp-11549 |
| Pd2V | [2 1 2] | -0.41 | mp-11549 |
| Pd3V | [1 0 0] | -0.4 | mp-873 |
| Pd3V | [1 0 1] | -0.34 | mp-873 |
| Pd3V | [1 1 0] | -0.32 | mp-873 |
| Pd3V | [2 1 1] | -0.4 | mp-568711 |
| Pd3V | [2 1 1] | -0.33 | mp-568711 |
| Pd3V | [2 2 1] | -0.39 | mp-568711 |
| Pd6V2 | [1 0 0] | -0.46 | mp-979980 |
| Pd6V2 | [1 0 2] | -0.24 | mp-979980 |
| Pd6V2 | [1 1 1] | -0.37 | mp-979980 |
| Pt | [1 1 1] | -0.36 | mp-126 |
| Pt7Cu | [1 0 0] | -0.44 | mp-12608 |
| Pt7Cu | [1 0 0] | -0.36 | mp-12608 |
| PtCu3 | [1 1 0] | -0.34 | mp-12086 |
| PtCu3 | [1 1 0] | -0.28 | mp-12086 |
| PtCu3 | [1 1 1] | -0.32 | mp-12086 |
| PtCu3 | [2 1 1] | -0.27 | mp-12086 |
| PtCu3 | [2 2 1] | -0.25 | mp-12086 |
| Pt2CuIn | [1 0 0] | -0.35 | mp-639659 |
| Pt2CuIn | [2 0 1] | -0.44 | mp-639659 |
| Pt2CuIn | [2 1 1] | -0.46 | mp-639659 |
| Pt2FeCu | [0 0 1] | -0.31 | mp-3702 |
| Pt2FeCu | [1 0 1] | -0.42 | mp-3702 |
| Pt13In9 | [1 0 0] | -0.44 | mp-571060 |
| Pt13In9 | [2 0 -1] | -0.37 | mp-571060 |
| Pt3In | [1 0 0] | -0.46 | mp-20516 |
| Pt3In | [1 0 0] | -0.25 | mp-20516 |
| Pt5In5 | [0 0 1] | -0.36 | mp-510438 |
| Pt5In5 | [1 1 -1] | -0.3 | mp-510438 |
| Pt8Ti | [2 1 1] | -0.38 | mp-30852 |
| Pt2V | [0 0 1] | -0.35 | mp-12108 |
| Pt2V | [0 1 2] | -0.27 | mp-12108 |
| Pt2V | [1 1 0] | -0.45 | mp-12108 |
| Pt2V2 | [1 0 0] | -0.45 | mp-1017531 |
| Pt3V | [0 0 1] | -0.44 | mp-2705 |
| Pt3V | [0 0 1] | -0.21 | mp-2705 |
| Pt3V | [1 1 2] | -0.26 | mp-2705 |
| Pt3V | [2 1 0] | -0.31 | mp-372 |
| Re2Al12 | [0 1 0] | -0.17 | mp-16528 |
| Re2Al12 | [1 1 0] | -0.46 | mp-16528 |
| ReAl12 | [1 0 0] | -0.22 | mp-1648 |
| Re6Pt2 | [0 0 1] | -0.46 | mp-862589 |
| Re4Si4 | [1 0 0] | -0.44 | mp-7948 |
| Rh | [1 0 0] | -0.45 | mp-74 |
| Rh | [1 1 1] | -0.39 | mp-74 |
| Rh4Al18 | [0 0 1] | -0.4 | mp-1645 |
| Rh4Al18 | [0 0 1] | -0.2 | mp-1645 |
| Rh4Al18 | [0 1 1] | -0.37 | mp-1645 |
| Rh4Al18 | [1 0 -1] | -0.19 | mp-1645 |
| Rh4Al18 | [1 0 0] | -0.35 | mp-1645 |
| Rh4Al18 | [1 0 0] | -0.3 | mp-1645 |
| Rh4Al18 | [1 0 1] | -0.36 | mp-1645 |
| Rh4Al18 | [1 1 0] | -0.31 | mp-1645 |
| Rh4Al18 | [1 1 0] | -0.3 | mp-1645 |
| Rh8Al20 | [0 0 1] | -0.45 | mp-1791 |
| Rh8Al20 | [1 1 0] | -0.42 | mp-1791 |
| RhAl | [1 0 0] | -0.37 | mp-364 |
| RhAl | [1 1 0] | -0.26 | mp-364 |
| RhAl | [2 1 0] | -0.18 | mp-364 |
| RhAl | [2 1 1] | -0.17 | mp-364 |
| RhAl | [2 2 1] | -0.34 | mp-364 |
| Rh2AlTi | [2 1 0] | -0.45 | mp-866153 |
| Rh2AlTi | [2 1 0] | -0.41 | mp-866153 |
| Rh2CoSn | [1 0 0] | -0.42 | mp-1018085 |
| Rh2CuGa | [1 1 1] | -0.47 | mp-862485 |
| Rh2CuV | [1 0 0] | -0.43 | mp-979910 |
| Rh2CuV | [1 1 1] | -0.37 | mp-979910 |
| Rh2CuV | [2 1 0] | -0.42 | mp-979910 |
| Rh2FeAl | [2 1 0] | -0.42 | mp-861953 |
| Rh6Ga10 | [0 0 1] | -0.23 | mp-30923 |
| Rh6Ga10 | [1 0 -2] | -0.29 | mp-30923 |
| Rh6Ga10 | [1 2 -1] | -0.2 | mp-30923 |
| RhGa | [1 0 0] | -0.37 | mp-2444 |
| RhGa | [1 0 0] | -0.36 | mp-2444 |
| Rh4In12 | [1 0 0] | -0.28 | mp-18614 |
| Rh4In12 | [1 0 1] | -0.28 | mp-18614 |
| Rh4In12 | [2 1 1] | -0.31 | mp-18614 |
| Rh3Pt | [1 0 0] | -0.45 | mp-974370 |
| Rh3Pt | [1 0 0] | -0.39 | mp-974370 |
| Rh3Pt | [1 0 0] | -0.34 | mp-974376 |
| Rh3Pt | [1 0 1] | -0.42 | mp-974376 |
| Rh3Pt | [1 0 1] | -0.39 | mp-974376 |
| Rh3Pt | [1 1 1] | -0.43 | mp-974370 |
| Rh3Pt | [2 1 0] | -0.41 | mp-974376 |
| RhPt3 | [0 0 1] | -0.41 | mp-974616 |
| RhPt3 | [1 1 2] | -0.37 | mp-974616 |
| Rh3Sn | [1 1 2] | -0.42 | mp-978974 |
| Rh4Sn4 | [1 0 0] | -0.23 | mp-317 |
| Rh4Sn4 | [1 1 0] | -0.37 | mp-317 |
| Rh4Sn4 | [1 1 1] | -0.33 | mp-317 |
| Rh4Sn4 | [2 1 0] | -0.25 | mp-317 |
| Rh2SnTi | [1 0 0] | -0.34 | mp-865707 |
| Rh2SnTi | [2 1 0] | -0.45 | mp-865707 |
| Rh2V2 | [0 0 1] | -0.34 | mp-971751 |
| Rh2V2 | [1 0 0] | -0.32 | mp-1251 |
| Rh2V2 | [2 2 1] | -0.46 | mp-1251 |
| Rh2V2 | [2 2 1] | -0.41 | mp-1251 |
| Rh2V6 | [1 1 0] | -0.44 | mp-1578 |
| Rh3V | [1 0 0] | -0.43 | mp-1185 |
| Ru2 | [1 0 0] | -0.44 | mp-33 |
| Ru2As4 | [1 2 0] | -0.19 | mp-766 |
| Ru2As4 | [2 1 0] | -0.43 | mp-766 |
| RuCoAl2 | [1 1 1] | -0.41 | mp-862695 |
| Ru4In12 | [1 0 0] | -0.31 | mp-672326 |
| Ru2SiGa | [2 1 0] | -0.35 | mp-865615 |
| Ru2Zn6 | [1 0 1] | -0.46 | mp-1380 |
| Sb2Al2 | [1 1 1] | -0.45 | mp-1018100 |
| Sb2Al2 | [1 1 1] | -0.28 | mp-1018100 |
| Sb2Al2 | [2 1 1] | -0.35 | mp-1018100 |
| Sb2Al2 | [2 1 2] | -0.32 | mp-1018100 |
| SbAl | [1 1 1] | -0.38 | mp-2624 |
| SbAl | [2 2 1] | -0.34 | mp-2624 |
| Sb4Co2 | [2 1 2] | -0.3 | mp-9835 |
| Sb8Co4 | [2 1 0] | -0.2 | mp-755 |
| Sb8Co4 | [2 1 1] | -0.22 | mp-755 |
| Sb2CuNi | [1 0 0] | -0.36 | mp-11834 |
| Sb2CuNi | [1 0 1] | -0.29 | mp-11834 |
| Sb2Ga2 | [2 1 1] | -0.24 | mp-1018059 |
| SbGa | [2 1 0] | -0.31 | mp-1156 |
| Sb8Ir4 | [1 1 0] | -0.37 | mp-1247 |
| SbMnRh | [2 1 0] | -0.37 | mp-4846 |
| SbMnRh2 | [1 1 2] | -0.42 | mp-571163 |
| SbMnRu2 | [2 1 0] | -0.41 | mp-864957 |
| Sb2Ni2 | [1 0 0] | -0.43 | mp-810 |
| Sb2Ni2 | [1 1 1] | -0.25 | mp-810 |
| Sb2Ni2 | [1 1 1] | -0.21 | mp-810 |
| Sb2Ni2 | [2 1 1] | -0.23 | mp-810 |
| Sb2Ni2 | [2 1 1] | -0.21 | mp-810 |
| Sb4Os2 | [0 1 2] | -0.43 | mp-2695 |
| Sb4Os2 | [0 1 2] | -0.4 | mp-2695 |
| Sb2Pt2 | [1 0 0] | -0.33 | mp-2845 |
| SbPt7 | [1 0 0] | -0.33 | mp-1030 |
| SbPt7 | [1 1 1] | -0.29 | mp-1030 |
| Sb4Rh4 | [1 0 0] | -0.2 | mp-20619 |
| Sb4Rh8 | [1 0 0] | -0.35 | mp-21359 |
| Sb4Rh8 | [2 0 1] | -0.42 | mp-21359 |
| Sb8Rh4 | [1 1 -2] | -0.41 | mp-2682 |
| Sb8Rh4 | [1 2 -1] | -0.2 | mp-2682 |
| Sb8Rh4 | [2 1 -1] | -0.21 | mp-2682 |
| SbRh2Cu | [2 1 0] | -0.44 | mp-867753 |
| Sb8Si8Pt8 | [1 0 0] | -0.45 | mp-11152 |
| Sb8Si8Pt8 | [1 1 0] | -0.43 | mp-11152 |
| SbSiPt5 | [0 0 1] | -0.3 | mp-1025366 |
| SbSiPt5 | [1 0 0] | -0.31 | mp-1025366 |
| SbSiPt5 | [2 1 2] | -0.47 | mp-1025366 |
| Sb4V2 | [2 1 1] | -0.41 | mp-2851 |
| SiAgPt5 | [1 0 0] | -0.44 | mp-1025220 |
| SiAgPt5 | [1 0 1] | -0.44 | mp-1025220 |
| SiAgPt5 | [2 1 2] | -0.47 | mp-1025220 |
| Si2Co2Al | [1 1 0] | -0.41 | mp-10010 |
| Si2Co2Al | [1 1 1] | -0.42 | mp-10010 |
| Si2Co2Al | [2 1 0] | -0.42 | mp-10010 |
| Si2Co2Al | [2 1 0] | -0.42 | mp-10010 |
| Si2Fe4 | [1 1 1] | -0.43 | mp-22787 |
| Si8Fe4Al12 | [1 1 0] | -0.38 | mp-505229 |
| Si8Fe6Al4 | [0 0 1] | -0.4 | mp-29111 |
| SiFe2Al | [1 1 1] | -0.37 | mp-867878 |
| Si2Ir6 | [0 0 1] | -0.3 | mp-1841 |
| Si2Ir6 | [2 1 1] | -0.47 | mp-1841 |
| Si4Ir4 | [0 1 1] | -0.44 | mp-1128 |
| Si2Mn6Al18 | [1 1 0] | -0.37 | mp-15819 |
| Si16Os8 | [0 0 1] | -0.47 | mp-17123 |
| SiOs2V | [2 1 0] | -0.46 | mp-865506 |
| SiOs2V | [2 1 0] | -0.45 | mp-865506 |
| Si3Pd6 | [1 0 1] | -0.19 | mp-697068 |
| Si4Pd12 | [0 0 1] | -0.34 | mp-20622 |
| Si4Pd12 | [0 1 1] | -0.25 | mp-20622 |
| Si4Pd12 | [1 0 0] | -0.31 | mp-20622 |
| Si4Pd12 | [1 0 2] | -0.35 | mp-20622 |
| Si4Pd12 | [1 0 2] | -0.32 | mp-20622 |
| Si4Pd12 | [1 2 0] | -0.33 | mp-20622 |
| Si4Pd12 | [2 1 0] | -0.31 | mp-20622 |
| Si2Pt6 | [0 1 0] | -0.42 | mp-13363 |
| Si2Pt6 | [2 0 -1] | -0.33 | mp-13363 |
| Si4Pt12 | [0 0 1] | -0.44 | mp-21163 |
| Si4Pt12 | [1 2 0] | -0.39 | mp-21163 |
| Si4Pt12 | [1 2 1] | -0.4 | mp-21163 |
| Si4Pt4 | [2 0 1] | -0.46 | mp-696 |
| SiPt2 | [1 1 2] | -0.44 | mp-1299 |
| SiPt5In | [1 0 0] | -0.41 | mp-1025370 |
| SiPt5In | [2 0 1] | -0.34 | mp-1025370 |
| SiPt5In | [2 1 0] | -0.4 | mp-1025370 |
| Si6Rh10 | [1 0 0] | -0.38 | mp-21012 |
| SiRh2Cu | [1 1 0] | -0.47 | mp-978532 |
| SiRh2Zn | [1 0 0] | -0.46 | mp-977384 |
| SiRh2Zn | [2 1 0] | -0.42 | mp-977384 |
| SiSnPt5 | [1 0 0] | -0.42 | mp-1025324 |
| SiSnPt5 | [1 1 1] | -0.45 | mp-1025324 |
| Si6V3 | [1 0 0] | -0.34 | mp-10711 |
| Si6V3 | [1 1 0] | -0.21 | mp-11190 |
| Si6V3 | [2 1 1] | -0.36 | mp-11190 |
| Si2W | [1 1 0] | -0.38 | mp-1620 |
| Si6W3 | [1 1 0] | -0.34 | mp-8939 |
| Sn2Cu2 | [1 0 0] | -0.39 | mp-10598 |
| Sn4Pd4 | [0 1 0] | -0.26 | mp-2369 |
| Sn4Pd4 | [1 0 1] | -0.17 | mp-2369 |
| Sn4Pd4 | [2 1 2] | -0.26 | mp-2369 |
| Sn4Pd8 | [1 0 1] | -0.28 | mp-1851 |
| Sn4Pd8 | [1 1 0] | -0.23 | mp-1851 |
| Sn4Pd8 | [1 1 2] | -0.24 | mp-1851 |
| Sn4Pd8 | [1 2 2] | -0.29 | mp-1851 |
| SnPd3 | [1 0 0] | -0.39 | mp-718 |
| SnPdTi | [2 1 0] | -0.46 | mp-961682 |
| Sn2Pt2 | [1 1 1] | -0.36 | mp-19856 |
| Sn2Pt2 | [2 1 0] | -0.17 | mp-19856 |
| SnPt3 | [1 0 0] | -0.46 | mp-20971 |
| Sn2Ti4 | [1 0 0] | -0.2 | mp-30875 |
| TiPd2In | [1 0 0] | -0.32 | mp-866168 |
| TiRh2In | [1 0 0] | -0.39 | mp-866170 |
| TiRh2In | [2 1 0] | -0.47 | mp-866170 |
| Zn2As4Sn2 | [1 0 0] | -0.38 | mp-5190 |
| Zn3Co | [1 1 2] | -0.2 | mp-971948 |
| Zn13Fe | [2 0 1] | -0.41 | mp-1722 |
| ZnPt3 | [1 0 0] | -0.45 | mp-30856 |
| ZnPt3 | [2 1 0] | -0.39 | mp-30856 |
| ZnPt3 | [2 1 0] | -0.38 | mp-30856 |
| Zn2RhPd | [2 1 0] | -0.43 | mp-864839 |
| ZnRh2V | [1 0 0] | -0.35 | mp-865487 |
| ZnRh2V | [2 1 0] | -0.45 | mp-865487 |
| ZnRh2V | [2 1 0] | -0.43 | mp-865487 |
| Zn3Ti | [2 2 1] | -0.34 | mp-21289 |