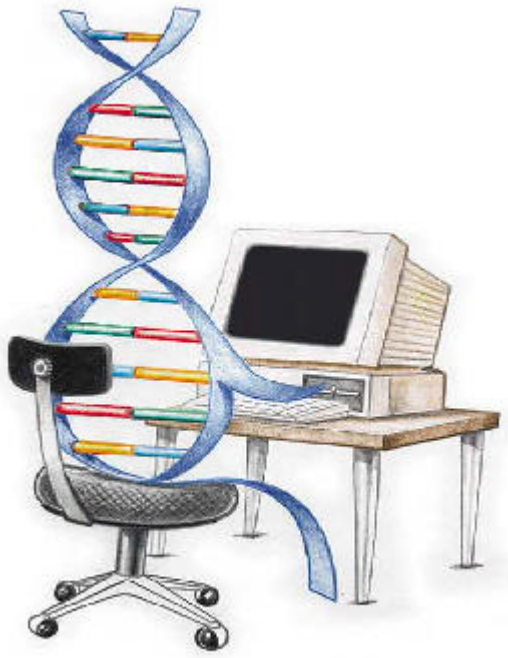
# Combined electronic structure calculations and evolutionary search for the most stable alloys



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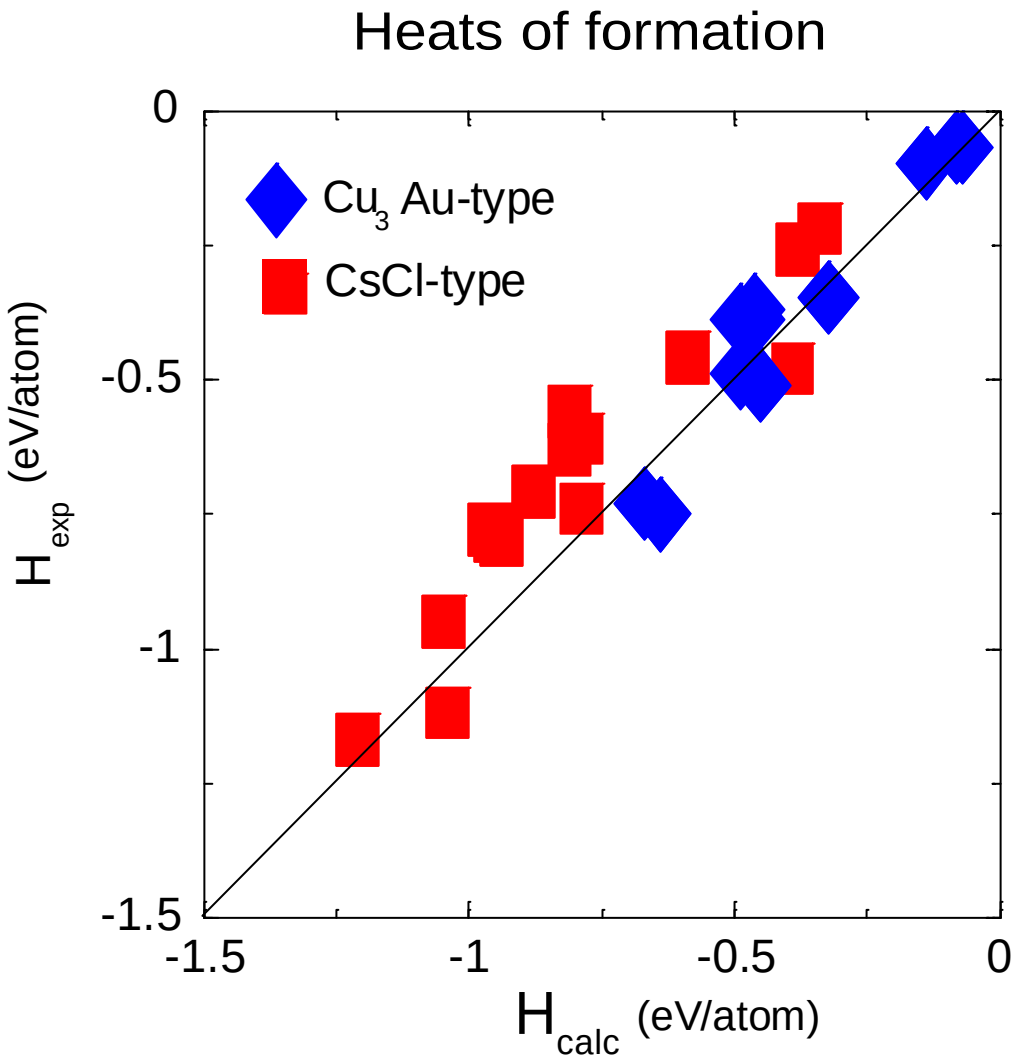
genetic

# Electronic structure Calculations

Linear Muffin-Tin orbitals (LMTO) method with multipole-corrected Atomic Sphere Approximation (ASA) and Generalized Gradient Approximation (GGA)

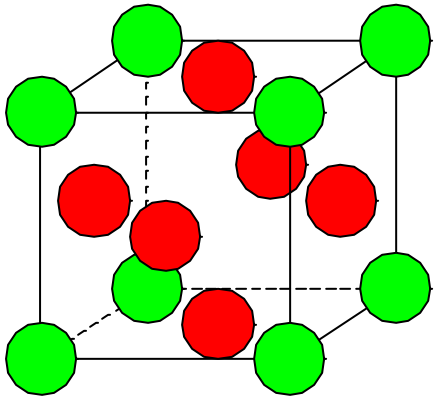
Experiments from "Cohesion in Metals", de Boer et al. (1988)



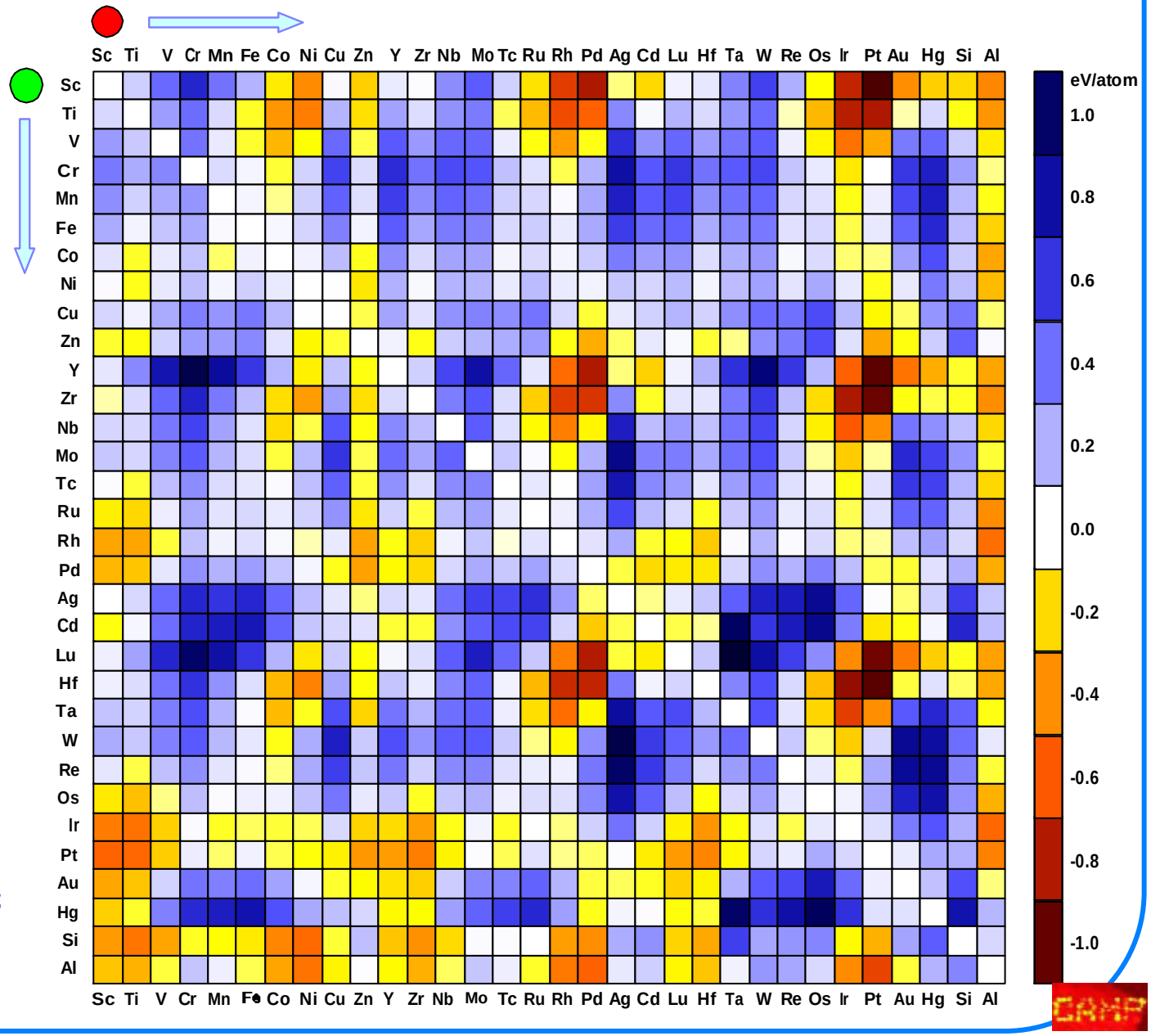
# Binary fcc alloys

All 992 different 1:3 combinations

Rugged landscape with many local minima



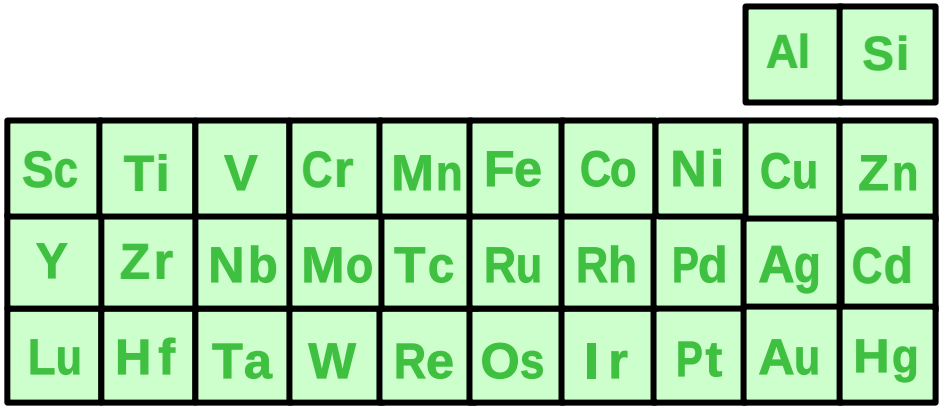
$L1_2$ ($Cu_3Au$) structure

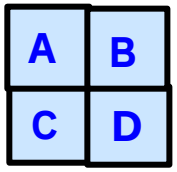


# Evolutionary Algorithm

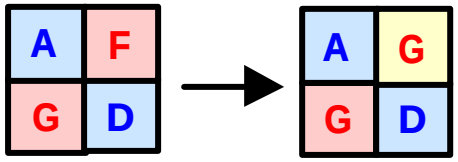
What do you need?

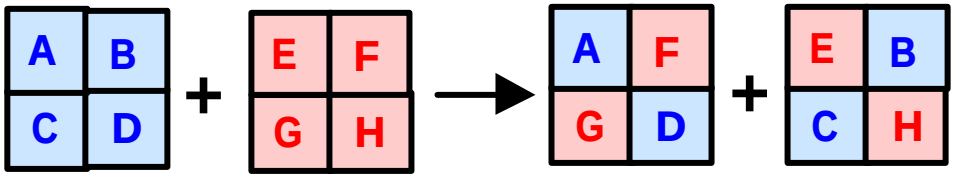
- Gene pool
- Individuals
- Selection scheme
- Mating scheme
- Mutation scheme



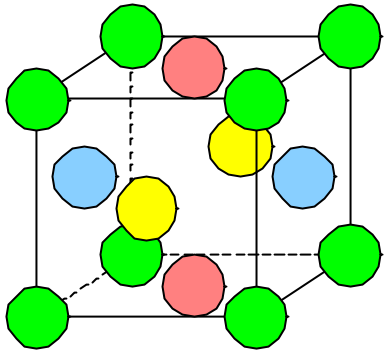

Initially the parents of a generation are chosen at random from the gene pool, then the parents are the best of the population



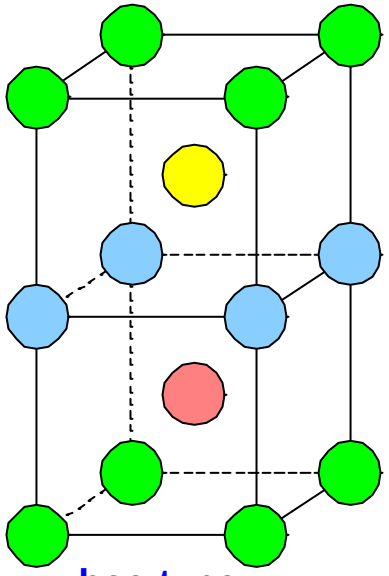



# Structure Optimization

- Four-atom unit cells
- One fcc and up to three bcc's per alloy: 192,016 possibilities
- Four to five volumes per alloy and per element to find the equilibrium
- Pick the structure with the lowest heat of formation stable againt decomposition into two-atom bcc structures

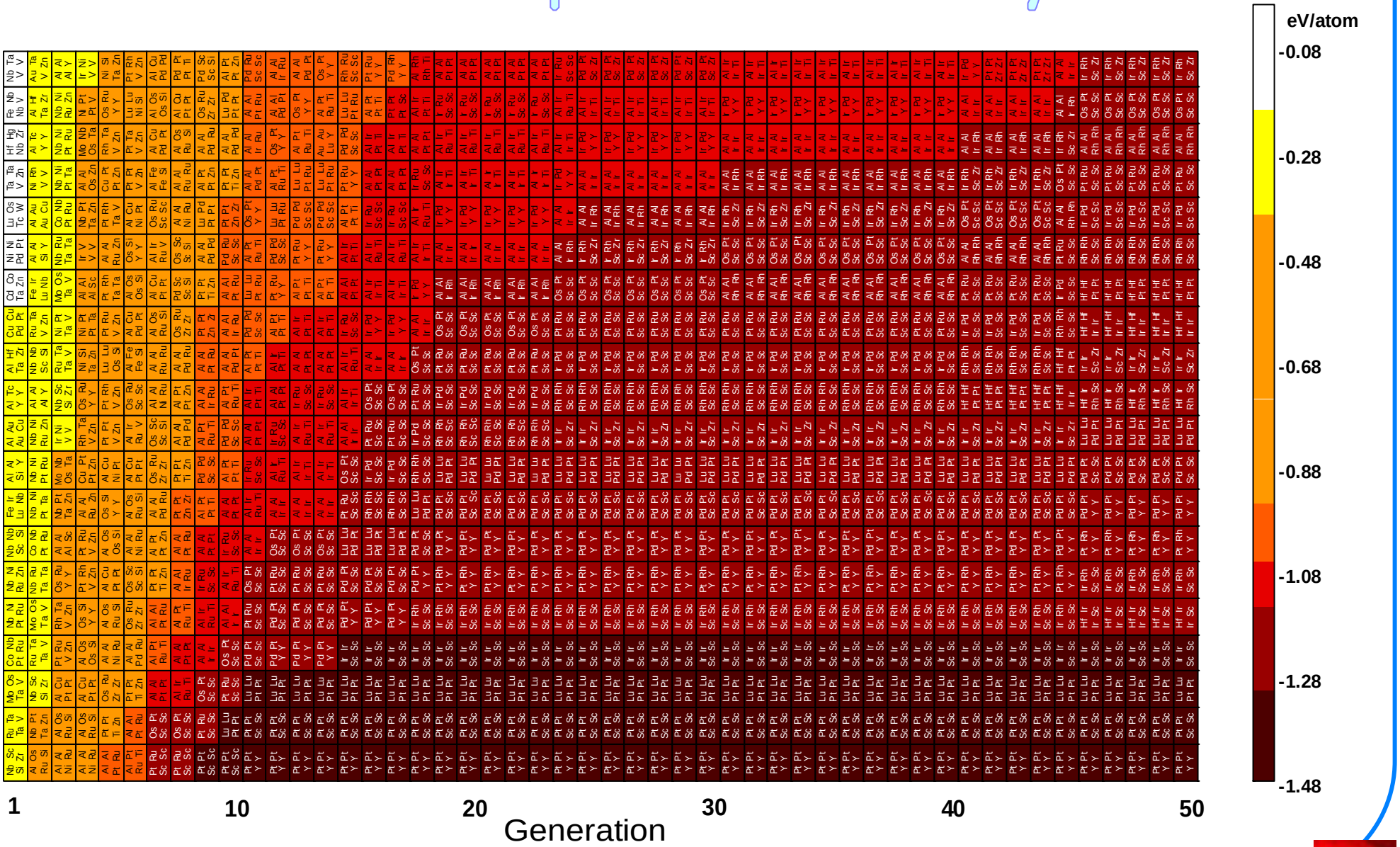


fcc-type



bcc-type

# Four-component alloys



# Identified alloys

| All | | fcc | | fcc excl. noble | | fcc excl. Si | |
|---|---|---|---|---|---|---|---|
| $Pt_2Y_2$ | -1.48 | $Pt_3Sc$ | -1.06 | $Si_2Ti_2$ | -0.57 | $AlNi_3$ | -0.49 |
| $Pt_2Sc_2$ | -1.47 | $HfPt_3$ | -1.03 | $NiSiTi_2$ | -0.55 | $Ni_3Ti$ | -0.46 |
| $Lu_2Pt_2$ | -1.41 | $Pt_3Y$ | -1.02 | $Si_2TaTi$ | -0.53 | $HfNi_3$ | -0.44 |
| $Ir_2Sc_2$ | -1.35 | $PdPt_2Sc$ | -0.99 | $Ni_3Si$ | -0.53 | $Al_2Ti_2$ | -0.43 |
| $HfIr_2Sc$ | -1.30 | $Pt_3Zr$ | -0.98 | $AlSiTi_2$ | -0.53 | $Al_3Sc$ | -0.43 |
| $IrRhSc_2$ | -1.29 | $HfPt_2Rh$ | -0.98 | $Ni_2SiTa$ | -0.53 | $Al_2Zr_2$ | -0.42 |
| $PtRhY_2$ | -1.27 | $PdPt_2Y$ | -0.97 | $CoNiSiTa$ | -0.52 | $Al_2ZnZr$ | -0.42 |
| $PdPtY_2$ | -1.27 | $HfPdPt_2$ | -0.96 | $NiSiTaTi$ | -0.51 | $Al_2Sc_2$ | -0.41 |
| $PdPtSc_2$ | -1.26 | $LuPt_3$ | -0.95 | $AlSiTaTi$ | -0.50 | $Ni_3Sc$ | -0.41 |
| $PdPtLu_2$ | -1.24 | $Pt_2RhSc$ | -0.94 | $Sc_2Si_2$ | -0.50 | $Al_3Zr$ | -0.40 |
| $HfIrRhSc$ | -1.23 | $NiPt_2Sc$ | -0.93 | $CoSiTaTi$ | -0.50 | $Al_2TiZn$ | -0.39 |
| $Ir_2ScZr$ | -1.23 | $Pt_2RhZr$ | -0.92 | $AlNi_3$ | -0.49 | $Al_2ScZn$ | -0.38 |
| $Hf_2Ir_2$ | -1.23 | $HfNiPt_2$ | -0.92 | $SiTi_3$ | -0.49 | $Al_3Ti$ | -0.38 |
| $Hf_2Pt_2$ | -1.21 | $LuPdPt_2$ | -0.92 | $Si_2Zr_2$ | -0.47 | $Co_3Ti$ | -0.38 |
| $Rh_2Sc_2$ | -1.21 | $PdPt_2Zr$ | -0.92 | $AlSc_2Si$ | -0.46 | $Ni_3Zr$ | -0.36 |
| $IrPdSc_2$ | -1.20 | $Pd_2PtSc$ | -0.91 | $Ni_3Ti$ | -0.46 | $Al_2NbTi$ | -0.36 |
| $PtRuSc_2$ | -1.19 | $HfIrPtRh$ | -0.90 | $NiSiTaZn$ | -0.46 | $Al_2CuTi$ | -0.35 |
| $Al_2Rh_2$ | -1.18 | $Pd_2PtY$ | -0.90 | $AlSiZr_2$ | -0.46 | $Al_2HfZn$ | -0.34 |
| $OsPtSc_2$ | -1.17 | $HfPtRh_2$ | -0.88 | $SiTi_2Zn$ | -0.45 | $Al_2CuZr$ | -0.34 |
| $IrRhScZr$ | -1.17 | $HfIr_3$ | -0.88 | $HfNi_3$ | -0.44 | $Al_3Lu$ | -0.34 |

table