Extra Credit: Prototype Search

The systems we chose are intermetallic binary compounds between rare-earth elements. Dshemuchadse *et al.* [1] showed that statistically there are several prototype structures that are favored. We chose 12 of the most common binary solids in ICSD[2]:

cP4-Cu_3Au	cF24-Cu_2Mg	hP12-$MgZn_2$	hP6-$CaCu_5$	oS8-TlI	oP16-Fe_3C
oP12-Co_2Si	oI12-KHg_2	cP8-Cr_3Si	hP8-Mg_3Cd	cF8-NaCl	tP2-AuCu

And the elements we have are:

Ce	Pr	Nd	Sm	Eu	Ho	Er	Tm	Yb	Lu

For pseudopotential, we used Perdew-Zunger[3] LDA calculated by Hartwigsen, Goedecker, and Hutter[4] (*.pz-sp-hgh.UPF in PWSCF) to cover the whole lanthanides. We missed some of them in our bash script, so there are only part of lanthanides in our calculations.

By combining two different element and one structure, we perform a high-throughput computation of ~1000 calculations to get a rough understanding of possible structures, and computed again using higher precision to confirm our results.

In http://oqmd.org/materials/composition/Ce-Pr-Nd-Sm-Eu-Ho-Er-Tm-Yb-Lu [5,6]. we can find that only Yb and Eu are found to form compounds, $\Delta H_f(\mathrm{YbEu}) = -0.009\ \mathrm{eV/atom}$. This indicates it is fair to calculate with only elements as competing phases. We can deal with Yb-Eu compounds we find competitive in a post process.

In both rough and fine calculations, elements and compounds are both calculated to get a comparable result. An example input file for a rough run is as follows:

```
&control
    calculation = 'vc-relax',
    restart_mode = 'from_scratch',
/
 &system
    ecutwfc = 40.0,
    ecutrho = 160.0
    occupations = 'smearing'
    smearing = 'gaussian'
    degauss = 0.1
 /
 &electrons
    diagonalization='cg',
    mixing_mode = 'plain',
    mixing_beta = 0.7,
    conv_thr =  1.0d-4
 /
 &ions
    ion_dynamics='bfgs'
/
 &cell
```

```
   cell_dynamics='bfgs'
 /
```

And for a fine run:

```
&control
    calculation = 'vc-relax',
    restart_mode = 'from_scratch',
/
 &system
    ecutwfc = 60.0,
    ecutrho = 240.0
    occupations = 'smearing'
    smearing = 'gaussian'
    degauss = 0.1
 /
 &electrons
    diagonalization='cg',
    mixing_mode = 'plain',
    mixing_beta = 0.7,
    conv_thr =  1.0d-6
 /
 &ions
    ion_dynamics='bfgs'
    trust_radius_min = 1.0d-2
/
 &cell
    cell_dynamics='bfgs'
    cell_factor=4.0
 /
```

K points are all generated by k_mesh.sh. For both rough and fine runs, KPPRA is set to 2000. The reason here is for a personal space there is only 80G available spaces. If submitting a series of 100 jobs with KPPRA=8000, disk would not be able to handle the output wavefunction files.

In the rough run, we calculated the ground state energy of each element (Ry/atom):

```
Ce  -77.25645273000000000000
Pr  -92.97235611000000000000
Nd  -110.44648968250000000000
Pm  -129.94919018000000000000
Sm  -151.60181335750000000000
Eu  -175.09375911000000000000
Gd  -201.38412745500000000000
Tb  -229.45233575333333333333
Dy  -260.60236380000000000000
Ho  -293.59931508000000000000
Er  -329.28071630500000000000
Tm  -367.45507422500000000000
Yb  -409.69363494000000000000
Lu  -453.55170270750000000000
```

Similarly, for compounds:

```
Ce    2    Pr    4    cF24-Cu2Mg    -525.96698460
Ce    4    Pr    8    cP4-Cu3Au
Ce    4    Pr    8    hP12-MgZn2
Ce    6    Pr    2    hP8-Mg3Cd    -649.36745848
Ce    8    Pr    4    oP12-Co2Si    -987.06620432
Ce    1    Pr    1    cF8-NaCl    -170.09522521
Ce    4    Pr    8    cP8-Cr3Si    -1052.31279648
Ce    1    Pr    5    hP6-CaCu5    -541.51589330
Ce    1    Pr    1    tP2-AuCu    -170.14663645
Ce    2    Nd    4    cF24-Cu2Mg    -596.19850498
Ce    3    Nd    1    cP4-Cu3Au    -341.97035832
Ce    4    Nd    8    hP12-MgZn2    -1192.25769563
Ce    6    Nd    2    hP8-Mg3Cd    -684.34245817
Ce    8    Nd    4    oP12-Co2Si    -1057.21571745
Ce    1    Nd    1    cF8-NaCl    -187.58211956
Ce    6    Nd    2    cP8-Cr3Si    -683.73664564
Ce    1    Nd    5    hP6-CaCu5    -629.29329679
Ce    1    Nd    1    tP2-AuCu    -187.64543503
Ce    2    Sm    4    cF24-Cu2Mg    -761.03988473
Ce    3    Sm    1    cP4-Cu3Au    -383.22471083
Ce    4    Sm    8    hP12-MgZn2    -1522.02646695
Ce    6    Sm    2    hP8-Mg3Cd    -766.82942767
Ce    8    Sm    4    oP12-Co2Si    -1222.13429011
Ce    1    Sm    1    cF8-NaCl    -228.84648565
Ce    6    Sm    2    cP8-Cr3Si    -766.26282751
Ce    1    Sm    5    hP6-CaCu5    -835.29293351
Ce    1    Sm    1    tP2-AuCu    -228.90113396
Ce    2    Eu    4    cF24-Cu2Mg    -854.84946085
......

"energy-prototype.out" 1230L, 59558C
```

By comparing the energy of elements and compounds, we get energy difference per atom:

$$E_{diff} = \frac{\left(n_{atom,1}E_{atom,1} + n_{atom,2}E_{atom,2}\right) - E_{compound}}{n_{atom,1} + n_{atom,1}}$$

All results for $E_{diff} > 0$ are as follows:

```
(   1)    8: E_diff = 0.024758002499993     Lu1Ce1     Lu Ce tP2-AuCu
(   2)   35: E_diff = 0.022099375000039     Lu1Sm1     Lu Sm tP2-AuCu
(   3)   38: E_diff = 0.098455179999746     Lu4Eu8     Lu Eu hP12-MgZn2
(   4)   43: E_diff = 0.085035102499887     Lu1Eu1     Lu Eu tP2-AuCu
(   5)   77: E_diff = 0.139037825000059     Lu2Ho2     Lu Ho tP2-AuCu
(   6)  110: E_diff = 0.024901142499971     Ce1Lu1     Ce Lu tP2-AuCu
(   7)  129: E_diff = 0.119725840000001     Ce2Sm4     Ce Sm cF24-Cu2Mg
(   8)  131: E_diff = 0.186149169999908     Ce4Sm8     Ce Sm hP12-MgZn2
(   9)  132: E_diff = 0.087084574999949     Ce6Sm2     Ce Sm hP8-Mg3Cd
(  10)  136: E_diff = 0.027413992500101     Ce1Sm5     Ce Sm hP6-CaCu5
(  11)  137: E_diff = 0.042867872500011     Ce1Sm1     Ce Sm tP2-AuCu
(  12)  140: E_diff = 0.741974410000012     Ce4Eu8     Ce Eu hP12-MgZn2
(  13)  141: E_diff = 0.232316220000030     Ce6Eu2     Ce Eu hP8-Mg3Cd
(  14)  143: E_diff = 0.076146669999986     Ce1Eu1     Ce Eu cF8-NaCl
(  15)  146: E_diff = 0.143063869999992     Ce1Eu1     Ce Eu tP2-AuCu
(  16)  150: E_diff = 0.099434419999852     Ce6Gd2     Ce Gd hP8-Mg3Cd
(  17)  155: E_diff = 0.053637325000011     Ce1Gd1     Ce Gd tP2-AuCu
(  18)  163: E_diff = 0.019228786666645     Ce1Tb1     Ce Tb tP2-AuCu
(  19)  174: E_diff = 0.029720859999998     Ce6Ho2     Ce Ho hP8-Mg3Cd
(  20)  179: E_diff = 0.054468680000014     Ce1Ho1     Ce Ho tP2-AuCu
(  21)  184: E_diff = 0.094610170000124     Ce2Er4     Ce Er oP12-Co2Si
(  22)  200: E_diff = 0.075512079999953     Ce6Yb2     Ce Yb hP8-Mg3Cd
(  23)  229: E_diff = 0.002181350000001     Pr4Sm8     Pr Sm hP12-MgZn2
(  24)  235: E_diff = 0.030716732500025     Pr1Sm1     Pr Sm tP2-AuCu
(  25)  239: E_diff = 0.065589459999956     Pr6Eu2     Pr Eu hP8-Mg3Cd
(  26)  244: E_diff = 0.066492989999972     Pr1Eu1     Pr Eu tP2-AuCu
(  27)  251: E_diff = 0.024382334999984     Pr1Gd1     Pr Gd tP2-AuCu
(  28)  336: E_diff = 0.004938509999874     Nd6Sm2     Nd Sm hP8-Mg3Cd
(  29)  345: E_diff = 0.131326715000000     Nd6Eu2     Nd Eu hP8-Mg3Cd
(  30)  350: E_diff = 0.090951797499997     Nd1Eu1     Nd Eu tP2-AuCu
(  31)  395: E_diff = 0.020351392500004     Nd1Er1     Nd Er tP2-AuCu
(  32)  414: E_diff = 0.014914769999905     Sm6Lu2     Sm Lu hP8-Mg3Cd
(  33)  419: E_diff = 0.022055075000026     Sm1Lu1     Sm Lu tP2-AuCu
(  34)  423: E_diff = 0.252355265000006     Sm6Ce2     Sm Ce hP8-Mg3Cd
(  35)  428: E_diff = 0.042687232500015     Sm1Ce1     Sm Ce tP2-AuCu
(  36)  437: E_diff = 0.030670082500023     Sm1Pr1     Sm Pr tP2-AuCu
(  37)  441: E_diff = 0.188909630000126     Sm6Nd2     Sm Nd hP8-Mg3Cd
(  38)  448: E_diff = 0.268498509999972     Sm4Eu8     Sm Eu hP12-MgZn2
(  39)  449: E_diff = 0.266044464999823     Sm6Eu2     Sm Eu hP8-Mg3Cd
(  40)  452: E_diff = 0.077759144999845     Sm6Eu2     Sm Eu cP8-Cr3Si
(  41)  454: E_diff = 0.090553892499997     Sm1Eu1     Sm Eu tP2-AuCu
(  42)  458: E_diff = 0.076877225000089     Sm6Gd2     Sm Gd hP8-Mg3Cd
(  43)  463: E_diff = 0.001272747500025     Sm1Gd1     Sm Gd tP2-AuCu
(  44)  481: E_diff = 0.002888032499982     Sm1Dy1     Sm Dy tP2-AuCu
(  45)  484: E_diff = 0.012063905000105     Sm6Ho2     Sm Ho hP8-Mg3Cd
(  46)  489: E_diff = 0.056043312500037     Sm1Ho1     Sm Ho tP2-AuCu
(  47)  493: E_diff = 0.048799445000213     Sm6Er2     Sm Er hP8-Mg3Cd
(  48)  496: E_diff = 0.084776147500008     Sm1Er1     Sm Er tP2-AuCu
(  49)  498: E_diff = 0.142724645000044     Sm6Tm2     Sm Tm hP8-Mg3Cd
(  50)  502: E_diff = 0.040772587500101     Sm1Tm1     Sm Tm tP2-AuCu
(  51)  511: E_diff = 0.012723202499956     Sm1Yb1     Sm Yb tP2-AuCu
```

(52)	515:	E_diff = 0.419683925000072	Eu6Lu2	Eu Lu	hP8-Mg3Cd
(53)	520:	E_diff = 0.085058702499964	Eu1Lu1	Eu Lu	tP2-AuCu
(54)	524:	E_diff = 0.626276970000163	Eu6Ce2	Eu Ce	hP8-Mg3Cd
(55)	526:	E_diff = 0.076138709999981	Eu1Ce1	Eu Ce	cF8-NaCl
(56)	527:	E_diff = 0.319187240000019	Eu6Ce2	Eu Ce	cP8-Cr3Si
(57)	529:	E_diff = 0.143449609999976	Eu1Ce1	Eu Ce	tP2-AuCu
(58)	533:	E_diff = 0.482984870000109	Eu6Pr2	Eu Pr	hP8-Mg3Cd
(59)	537:	E_diff = 0.067151189999947	Eu1Pr1	Eu Pr	tP2-AuCu
(60)	541:	E_diff = 0.551298515000099	Eu6Nd2	Eu Nd	hP8-Mg3Cd
(61)	544:	E_diff = 0.288147214999981	Eu6Nd2	Eu Nd	cP8-Cr3Si
(62)	546:	E_diff = 0.090962367500026	Eu1Nd1	Eu Nd	tP2-AuCu
(63)	553:	E_diff = 0.223972915000104	Eu6Sm2	Eu Sm	cP8-Cr3Si
(64)	555:	E_diff = 0.090537652499961	Eu1Sm1	Eu Sm	tP2-AuCu
(65)	559:	E_diff = 0.430816470000082	Eu6Gd2	Eu Gd	hP8-Mg3Cd
(66)	563:	E_diff = 0.065043295000009	Eu1Gd1	Eu Gd	tP2-AuCu
(67)	567:	E_diff = 0.357192093333424	Eu6Tb2	Eu Tb	hP8-Mg3Cd
(68)	572:	E_diff = 0.054313956666647	Eu1Tb1	Eu Tb	tP2-AuCu
(69)	579:	E_diff = 0.049972930000195	Eu6Dy2	Eu Dy	cP8-Cr3Si
(70)	581:	E_diff = 0.096805600000039	Eu1Dy1	Eu Dy	tP2-AuCu
(71)	585:	E_diff = 0.568267520000063	Eu6Ho2	Eu Ho	hP8-Mg3Cd
(72)	588:	E_diff = 0.089863110000124	Eu6Ho2	Eu Ho	cP8-Cr3Si
(73)	594:	E_diff = 0.657118670000273	Eu6Er2	Eu Er	hP8-Mg3Cd
(74)	597:	E_diff = 0.064362840000285	Eu6Er2	Eu Er	cP8-Cr3Si
(75)	599:	E_diff = 0.169206224999982	Eu1Er1	Eu Er	tP2-AuCu
(76)	603:	E_diff = 0.570792790000041	Eu6Tm2	Eu Tm	hP8-Mg3Cd
(77)	608:	E_diff = 0.122976155000060	Eu1Tm1	Eu Tm	tP2-AuCu
(78)	612:	E_diff = 0.477125419999993	Eu6Yb2	Eu Yb	hP8-Mg3Cd
(79)	617:	E_diff = 0.091237910000018	Eu1Yb1	Eu Yb	tP2-AuCu
(80)	621:	E_diff = 0.064137705000121	Gd6Lu2	Gd Lu	hP8-Mg3Cd
(81)	635:	E_diff = 0.053165735000050	Gd1Ce1	Gd Ce	tP2-AuCu
(82)	639:	E_diff = 0.227575990000105	Gd6Pr2	Gd Pr	hP8-Mg3Cd
(83)	644:	E_diff = 0.024718014999962	Gd1Pr1	Gd Pr	tP2-AuCu
(84)	662:	E_diff = 0.001287917500065	Gd1Sm1	Gd Sm	tP2-AuCu
(85)	665:	E_diff = 0.245137890000024	Gd4Eu8	Gd Eu	hP12-MgZn2
(86)	671:	E_diff = 0.065026854999985	Gd1Eu1	Gd Eu	tP2-AuCu
(87)	679:	E_diff = 0.007435871666701	Gd1Tb1	Gd Tb	tP2-AuCu
(88)	693:	E_diff = 0.084491694999997	Gd1Ho1	Gd Ho	tP2-AuCu
(89)	697:	E_diff = 0.264057890000231	Gd6Er2	Gd Er	hP8-Mg3Cd
(90)	702:	E_diff = 0.094431240000063	Gd1Er1	Gd Er	tP2-AuCu
(91)	706:	E_diff = 0.215005020000035	Gd6Tm2	Gd Tm	hP8-Mg3Cd
(92)	711:	E_diff = 0.038172580000037	Gd1Tm1	Gd Tm	tP2-AuCu
(93)	715:	E_diff = 0.041180230000009	Gd6Yb2	Gd Yb	hP8-Mg3Cd
(94)	765:	E_diff = 0.002876282499983	Dy1Sm1	Dy Sm	tP2-AuCu
(95)	768:	E_diff = 0.316306379999787	Dy4Eu8	Dy Eu	hP12-MgZn2
(96)	769:	E_diff = 0.169740539999793	Dy6Eu2	Dy Eu	hP8-Mg3Cd
(97)	774:	E_diff = 0.096781899999996	Dy1Eu1	Dy Eu	tP2-AuCu
(98)	778:	E_diff = 0.039127280000002	Dy6Gd2	Dy Gd	hP8-Mg3Cd
(99)	783:	E_diff = 0.050076065000042	Dy1Gd1	Dy Gd	tP2-AuCu
(100)	792:	E_diff = 0.024162696666679	Dy1Tb1	Dy Tb	tP2-AuCu
(101)	842:	E_diff = 0.055603670000039	Ho1Ce1	Ho Ce	tP2-AuCu
(102)	863:	E_diff = 0.011687064999933	Ho6Sm2	Ho Sm	hP8-Mg3Cd
(103)	871:	E_diff = 0.444605690000117	Ho4Eu8	Ho Eu	hP12-MgZn2
(104)	872:	E_diff = 0.228622589999759	Ho6Eu2	Ho Eu	hP8-Mg3Cd

```
( 105)  877: E_diff = 0.149064319999979     Ho1Eu1     Ho Eu tP2-AuCu
( 106)  881: E_diff = 0.030356119999851     Ho6Gd2     Ho Gd hP8-Mg3Cd
( 107)  886: E_diff = 0.084478755000021     Ho1Gd1     Ho Gd tP2-AuCu
( 108)  962: E_diff = 0.020337982499996     Er1Nd1     Er Nd tP2-AuCu
( 109)  973: E_diff = 0.497898779999559     Er4Eu8     Er Eu hP12-MgZn2
( 110)  979: E_diff = 0.169205014999989     Er1Eu1     Er Eu tP2-AuCu
( 111)  985: E_diff = 0.004614270000047     Er1Gd1     Er Gd cF8-NaCl
( 112)  988: E_diff = 0.094476540000073     Er1Gd1     Er Gd tP2-AuCu
( 113)  997: E_diff = 0.018214591666720     Er1Tb1     Er Tb tP2-AuCu
( 114)  1070: E_diff = 0.040793987500024     Tm1Sm1     Tm Sm tP2-AuCu
( 115)  1073: E_diff = 0.293357240000205     Tm4Eu8     Tm Eu hP12-MgZn2
( 116)  1161: E_diff = 0.312951334999980     Yb2Nd2     Yb Nd tP2-AuCu
( 117)  1173: E_diff = 0.082106890000432     Yb4Eu8     Yb Eu hP12-MgZn2
( 118)  1179: E_diff = 0.091183440000009     Yb1Eu1     Yb Eu tP2-AuCu
```

We then proceeded to finer calculation conditions to confirm the above results.

For `ecutwfc = 60.0,ecutrho = 240.0`, some calculations of elements are unable to finish, with the error message which would not happen with the rough input specification:

```
from efermig : error #         1
internal error, cannot bracket Ef
```

Nonetheless, we can at least go with the elements with confirmed message of `JOB DONE`.

The result we get for single elements are:

```
Ce  -77.27227833000000000000
Pr  -92.95007257750000000000
Nd  -110.436118612500000000000
Pm  -130.062990472500000000000
Sm  -151.659816012500000000000
Eu  -176.661702530000000000000
Gd  -9999
Tb  -9999
Dy  -9999
Ho  -288.731082850000000000000
Er  -323.374635145000000000000
Tm  -361.174299725000000000000
Yb  -406.274165020000000000000
Lu  -456.544504022500000000000
```

Set total energy of element to -9999 make those elements unbeatable, to make sure our result are correct. Though they may not be the most result we could get.

Up to now, our calculations have given confirmed results of the below structures that are below the elements. Indeed, there are some duplicates, as well as the competing phase of YbEu (B2) existing on OQMD[5,6]. Excluding all them, we have:

```
(   1)     5: E_diff = 1.262996823749972     Lu1Ho1     Lu Ho tP2-AuCu
~~(   2)     7: E_diff = 0.028232915000009     Ce2Sm4     Ce Sm cF24-Cu2Mg~~
(   3)     8: E_diff = 0.030177731666678     Ce4Sm8     Ce Sm hP12-MgZn2
(   4)     9: E_diff = 0.010183260624984     Ce6Sm2     Ce Sm hP8-Mg3Cd
(   5)    10: E_diff = 0.004699776250031     Ce1Sm5     Ce Sm hP6-CaCu5
(   6)    11: E_diff = 0.026263803749998     Ce1Sm1     Ce Sm tP2-AuCu
(   7)    19: E_diff = 1.304697773749979     Ce6Ho2     Ce Ho hP8-Mg3Cd
(   8)    20: E_diff = 2.574789114999987     Ce1Ho1     Ce Ho tP2-AuCu
(   9)    21: E_diff = 2.056441747499984     Ce8Er4     Ce Er oP12-Co2Si
(  10)    22: E_diff = 0.976523171249994     Ce6Yb2     Ce Yb hP8-Mg3Cd
(  11)    23: E_diff = 0.026721835000008     Pr4Sm8     Pr Sm hP12-MgZn2
(  12)    24: E_diff = 0.034201470000014     Pr1Sm1     Pr Sm tP2-AuCu
(  13)    28: E_diff = 0.055524212500004     Nd6Sm2     Nd Sm hP8-Mg3Cd
(  14)    30: E_diff = 3.123027816249987     Nd1Er1     Nd Er tP2-AuCu
~~(  15)    32: E_diff = 0.026266313750000     Sm1Ce1     Sm Ce tP2-AuCu~~
(  16)    33: E_diff = 0.034200920000018     Sm1Pr1     Sm Pr tP2-AuCu
(  17)    39: E_diff = 2.561592693750015     Sm1Ho1     Sm Ho tP2-AuCu
(  18)    40: E_diff = 3.119075301249978     Sm1Er1     Sm Er tP2-AuCu
(  19)    41: E_diff = 3.309266736249981     Sm1Tm1     Sm Tm tP2-AuCu
```

```
(  20)   42: E_diff = 1.867669228750003     Sm1Yb1     Sm Yb tP2-AuCu
(  21)   57: E_diff = 0.207405843749967     Eu6Ho2     Eu Ho cP8-Cr3Si
(  22)   58: E_diff = 0.485146618749980     Eu6Er2     Eu Er cP8-Cr3Si
(  23)   59: E_diff = 2.424655897499974     Eu1Er1     Eu Er tP2-AuCu
(  24)   60: E_diff = 2.612227857499988     Eu1Tm1     Eu Tm tP2-AuCu
(  25)   61: E_diff = 1.167773300000022     Eu1Yb1     Eu Yb tP2-AuCu
(  26)   76: E_diff = 2.574825314999998     Ho1Ce1     Ho Ce tP2-AuCu
(  27)   77: E_diff = 3.849487016875031     Ho6Sm2     Ho Sm hP8-Mg3Cd
(  28)   78: E_diff = 0.779497545833313     Ho4Eu8     Ho Eu hP12-MgZn2
(  29)   79: E_diff = 3.508098486249992     Ho6Eu2     Ho Eu hP8-Mg3Cd
(  30)   80: E_diff = 1.873103444999998     Ho1Eu1     Ho Eu tP2-AuCu
(  31)   82: E_diff = 3.123025931249970     Er1Nd1     Er Nd tP2-AuCu
(  32)   83: E_diff = 1.151460360833312     Er4Eu8     Er Eu hP12-MgZn2
(  33)   84: E_diff = 2.424658102499990     Er1Eu1     Er Eu tP2-AuCu
(  34)   88: E_diff = 3.309264716249970     Tm1Sm1     Tm Sm tP2-AuCu
(  35)   89: E_diff = 1.278974336666655     Tm4Eu8     Tm Eu hP12-MgZn2
(  36)   90: E_diff = 1.893020273749983     Yb1Nd1     Yb Nd tP2-AuCu
(  37)   91: E_diff = 0.309837560000005     Yb4Eu8     Yb Eu hP12-MgZn2
(  38)   92: E_diff = 1.167774604999977     Yb1Eu1     Yb Eu tP2-AuCu
```

There are 7 of them that are excluded, leaving at least 31 prototype search results that have beaten the current results in OQMD[5,6], according to the current selection of pseudopotential, K points, cutoff energy, etc. The above results have been confirmed by `JOB DONE` in both elements and compounds, so we believe they are sound results. For raw calculation data, please visit our GitHub page: https://github.com/PureHyd/MSE458_Final.

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