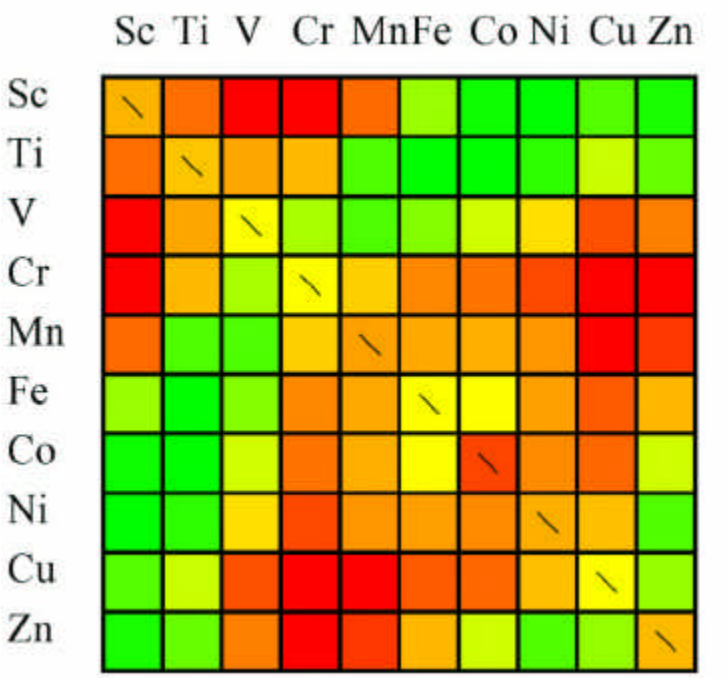
CAMP Alloy Database

http://databases.fysik.dtu.dk/

Hans L. Skriver



Center for Atomic-scale Materials Physics CAMP-DTU Lyngby

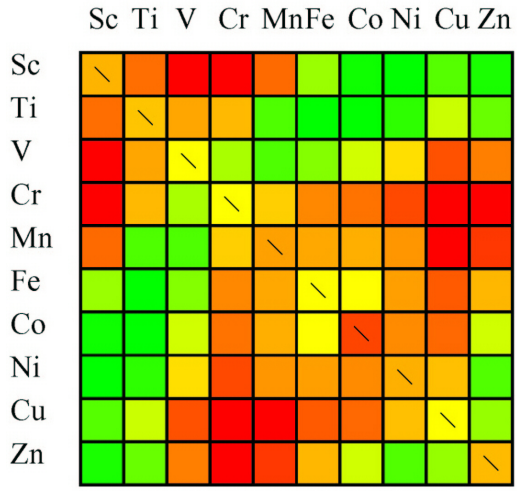
Front page Visitors

Welcome to Databases at CAMP

This website provides access to several databases containing scientific information about materials.

Choose the database you would like to search below:

- Alloys - hlsDB



Maintained by: DBwebmaster@fysik.dtu.dk

About databases.fysik.dtu.dk

The hls Alloy Database

This database have been made by Hans L. Skriver, who also maintains and expands it. Use the drop-down boxes to select the alloy(s) of interest, e.g., AgCu. To find all the possibilities search also for CuAg.
At least one element must be selected.

1. element: Co 2. element: Ti

Structure: <All>

Reset Search

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The hls Alloy Database

Search again:

1. element: Au 2. element: Cu

Structure: <All>

Reset Search

Click on alloy name to download equation of state file		Heat of Formation [eV/atom]		
Alloy name	**Structure**	**LDA**	**GGA**	**LAG**
Co_1Ti_1	B1	0,2547	0,2491	0,2407
Co_1Ti_1	B2	-0,4488	-0,3789	-0,4160
Co_4Ti_4	B20	-0,0721	-0,0392	-0,0618
Co_1Ti_3	DO3	-0,1415	-0,0721	-0,1054
Co_1Ti_3	DO22	0,0227	0,0573	0,0395
Co_1Ti_1	L10	-0,1745	-0,1107	-0,1442
Co_1Ti_1	L11	0,0301	0,0930	0,0592
Co_1Ti_3	L12	-0,0087	0,0219	0,0055
Co_2Ti_2	B11i	-0,0506	-0,0418	-0,0456
Alloy name	**Structure**	**Heat of Formation [eV/atom]**		

```
Fhndlr:   Program: EQOS, Version: HLS 25 Nov 2002                TM: 07:01
          isno=  0                                               10-Dec-02

          KGRN: Code=KKR-SCA Lmax=d Core=Soft-core-A BZ=sc NK= 455
          Job=CoTi_B2 isno=  0 AFM=F XC=Perdew-Wang-96-LDA Struc=B2
          it mmt nta Atom  Conc(it,ita):
          1   1   1  Co  1.0000
          2   1   1  Ti  1.0000

          Ground state parameters: LDA


          Sws_eq =        2.717070 Bohr;       Vol    =   84.02 Bohr**3
          Sws_exp=        2.850200 Bohr;       Rho    =    7.12 g/cm3
          E_eq   =    -2243.185269 Ry/atom;    E_form =   -0.032986 Ry/atom
          Bmod   =        1.989785 Mbar;       Bmod   =  198.98 GPa
          dB/dP  =        4.430151             Gamma  =    1.7151
          Error  =        0.000057 Ry(rms);    Alpha  =    9.45E-6 at 300.K

          Ground state parameters: GGA


          Sws_eq =        2.785133 Bohr;       Vol    =   90.50 Bohr**3
          Sws_exp=        2.850200 Bohr;       Rho    =    6.61 g/cm3
          E_eq   =    -2247.309966 Ry/atom;    E_form =   -0.027849 Ry/atom
          Bmod   =        1.623993 Mbar;       Bmod   =  162.40 GPa
          dB/dP  =        4.371997             Gamma  =    1.6860
          Error  =        0.000090 Ry(rms);    Alpha  =   10.75E-6 at 300.K

          Ground state parameters: LAG


          Sws_eq =        2.752887 Bohr;       Vol    =   87.39 Bohr**3
          Sws_exp=        2.850200 Bohr;       Rho    =    6.85 g/cm3
          E_eq   =    -2244.128127 Ry/atom;    E_form =   -0.030573 Ry/atom
          Bmod   =        1.769018 Mbar;       Bmod   =  176.90 GPa
          dB/dP  =        4.355722             Gamma  =    1.6779
          Error  =        0.000068 Ry(rms);    Alpha  =   10.09E-6 at 300.K


Eqos:     The formation energies [Ry/atom]

          S[au]            LDA            GGA            LAG
         2.850200      -0.022365      -0.025403      -0.025160
         2.900200      -0.014152      -0.021189      -0.019145
         2.800200      -0.028679      -0.027768      -0.029285
         2.750200      -0.032317      -0.027203      -0.030639
         2.700200      -0.032796      -0.023203      -0.028733
         2.650200      -0.029540      -0.015158      -0.022981
         2.600200      -0.021921      -0.002424      -0.012756
```

The hls Alloy Database

Search again:

1. element: <Select> 2. element: <Select>

Structure: <All>

Reset Search

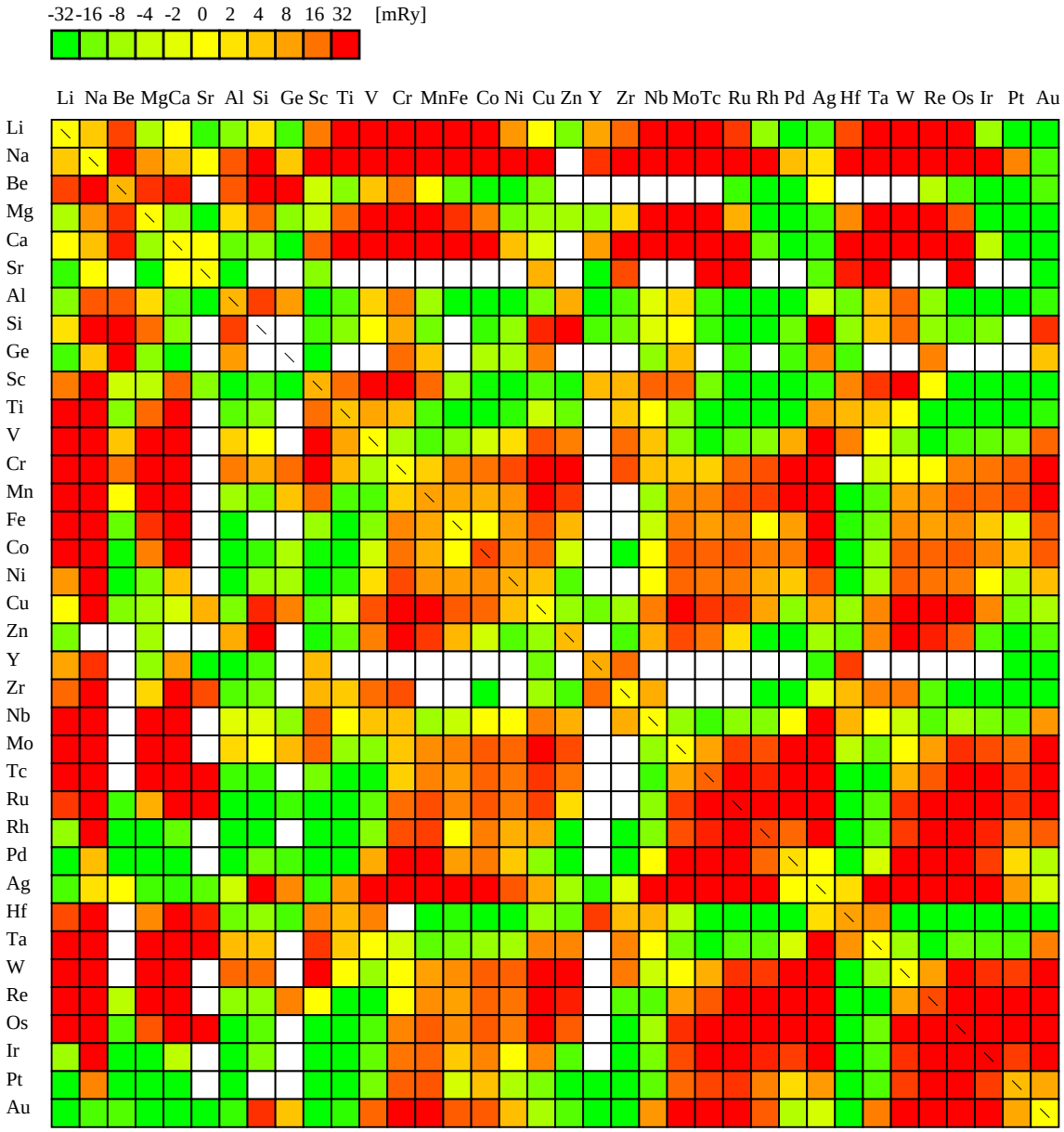
Click on alloy name to download equation of state file		Heat of Formation [eV/atom]		
Alloy name	**Structure**	**LDA**	**GGA**	**LAG**
Au_1Cu_1	B1	0,4986	0,3814	0,4237
Au_1Cu_1	B2	-0,0956	-0,0864	-0,0930
Au_4Cu_4	B20	0,0906	0,0567	0,0666
Au_1Cu_1	B27	1,4693	1,1166	1,2310
Au_2Cu_4	C15	0,1555	0,1308	0,1379
Au_1Cu_3	DO3	-0,0261	-0,0280	-0,0304
Au_1Cu_3	DO22	-0,0480	-0,0496	-0,0525
Au_1Cu_1	L10	-0,0445	-0,0474	-0,0512
Au_1Cu_1	L11	0,0678	0,0413	0,0465
Au_1Cu_3	L12	-0,0512	-0,0514	-0,0548
Au_2Cu_2	B11i	0,1364	0,0914	0,1032
Alloy name	**Structure**	**Heat of Formation [eV/atom]**		

```
Fhndlr:   Program: EQOS, Version: HLS 11 Dec 2002                TM: 15:37
          isno=  0                                               11-Dec-02

          KGRN: Code=KKR-SCA Lmax=d Core=Soft-core-A BZ=fcc NK= 505
          Job=AuCu_B1 isno=  0 AFM=P XC=Perdew-Wang-96-LDA Struc=B1
          it mmt nta Atom  Conc(it,ita):
          1   1   1  Au  1.0000
          2   1   1  Cu  1.0000

          Ground state parameters: LDA


          Sws_eq =        2.992769 Bohr;       Vol    =  112.28 Bohr**3
          Sws_exp=        2.850700 Bohr;       Rho    =   13.00 g/cm3
          E_eq   =   -20690.095952 Ry/atom;    E_form =    0.036649 Ry/atom
          Bmod   =        1.284019 Mbar;       Bmod   =  128.40 GPa
          dB/dP  =        6.375697             Gamma  =    2.6878
          Error  =        0.000020 Ry(rms);    Alpha  =   19.33E-6 at 300.K

          Ground state parameters: GGA


          Sws_eq =        3.090191 Bohr;       Vol    =  123.61 Bohr**3
          Sws_exp=        2.850700 Bohr;       Rho    =   11.80 g/cm3
          E_eq   =   -20703.158221 Ry/atom;    E_form =    0.028033 Ry/atom
          Bmod   =        0.870254 Mbar;       Bmod   =   87.03 GPa
          dB/dP  =        5.613892             Gamma  =    2.3069
          Error  =        0.000019 Ry(rms);    Alpha  =   22.35E-6 at 300.K

          Ground state parameters: LAG


          Sws_eq =        3.049444 Bohr;       Vol    =  118.78 Bohr**3
          Sws_exp=        2.850700 Bohr;       Rho    =   12.28 g/cm3
          E_eq   =   -20692.496624 Ry/atom;    E_form =    0.031141 Ry/atom
          Bmod   =        0.988682 Mbar;       Bmod   =   98.87 GPa
          dB/dP  =        5.979564             Gamma  =    2.4898
          Error  =        0.000020 Ry(rms);    Alpha  =   22.15E-6 at 300.K



Eqos:     The formation energies [Ry/atom]

          S[au]            LDA            GGA            LAG
        3.000000       0.036641       0.031238       0.032137
        3.050000       0.038134       0.028652       0.031172
        2.950000       0.037642       0.036557       0.035695
        2.900000       0.041711       0.045214       0.042444
        3.100000       0.041397       0.028075       0.032060
        3.150000       0.046078       0.029138       0.034463
        3.200000       0.051971       0.031609       0.038160
```

```
Fhndlr:   Program: EQOS, Version: HLS 25 Nov 2002                TM: 12:46
          isno=  0                                               08-Dec-02

          KGRN: Code=KKR-SCA Lmax=d Core=Soft-core-A BZ=sc NK= 455
          Job=AuCu_B2 isno=  0 AFM=P XC=Perdew-Wang-96-LDA Struc=B2
          it mmt nta Atom  Conc(it,ita):
          1   1   1  Au  1.0000
          2   1   1  Cu  1.0000

          Ground state parameters: LDA


          Sws_eq =        2.838873 Bohr;       Vol    =   95.84 Bohr**3
          Sws_exp=        2.850700 Bohr;       Rho    =   15.23 g/cm3
          E_eq   =   -20690.139625 Ry/atom;    E_form =   -0.007023 Ry/atom
          Bmod   =        1.769335 Mbar;       Bmod   =  176.93 GPa
          dB/dP  =        6.047433             Gamma  =    2.5237
          Error  =        0.000016 Ry(rms);    Alpha  =   15.08E-6 at 300.K

          Ground state parameters: GGA


          Sws_eq =        2.922918 Bohr;       Vol    =  104.60 Bohr**3
          Sws_exp=        2.850700 Bohr;       Rho    =   13.95 g/cm3
          E_eq   =   -20703.192605 Ry/atom;    E_form =   -0.006351 Ry/atom
          Bmod   =        1.271098 Mbar;       Bmod   =  127.11 GPa
          dB/dP  =        5.375188             Gamma  =    2.1876
          Error  =        0.000011 Ry(rms);    Alpha  =   16.75E-6 at 300.K

          Ground state parameters: LAG


          Sws_eq =        2.885572 Bohr;       Vol    =  100.64 Bohr**3
          Sws_exp=        2.850700 Bohr;       Rho    =   14.50 g/cm3
          E_eq   =   -20692.534603 Ry/atom;    E_form =   -0.006838 Ry/atom
          Bmod   =        1.428806 Mbar;       Bmod   =  142.88 GPa
          dB/dP  =        5.665077             Gamma  =    2.3325
          Error  =        0.000011 Ry(rms);    Alpha  =   16.51E-6 at 300.K


Eqos:     The formation energies [Ry/atom]

          S[au]            LDA            GGA            LAG
        2.850700      -0.006952      -0.003583      -0.006169
        2.900700      -0.004820      -0.006115      -0.006728
        2.800700      -0.005992       0.002337      -0.002419
        2.750700      -0.001116       0.012490       0.005365
        2.950700      -0.000323      -0.005997      -0.004811
        3.000700       0.006037      -0.003759      -0.000929
        3.050700       0.013834       0.000158       0.004493
```

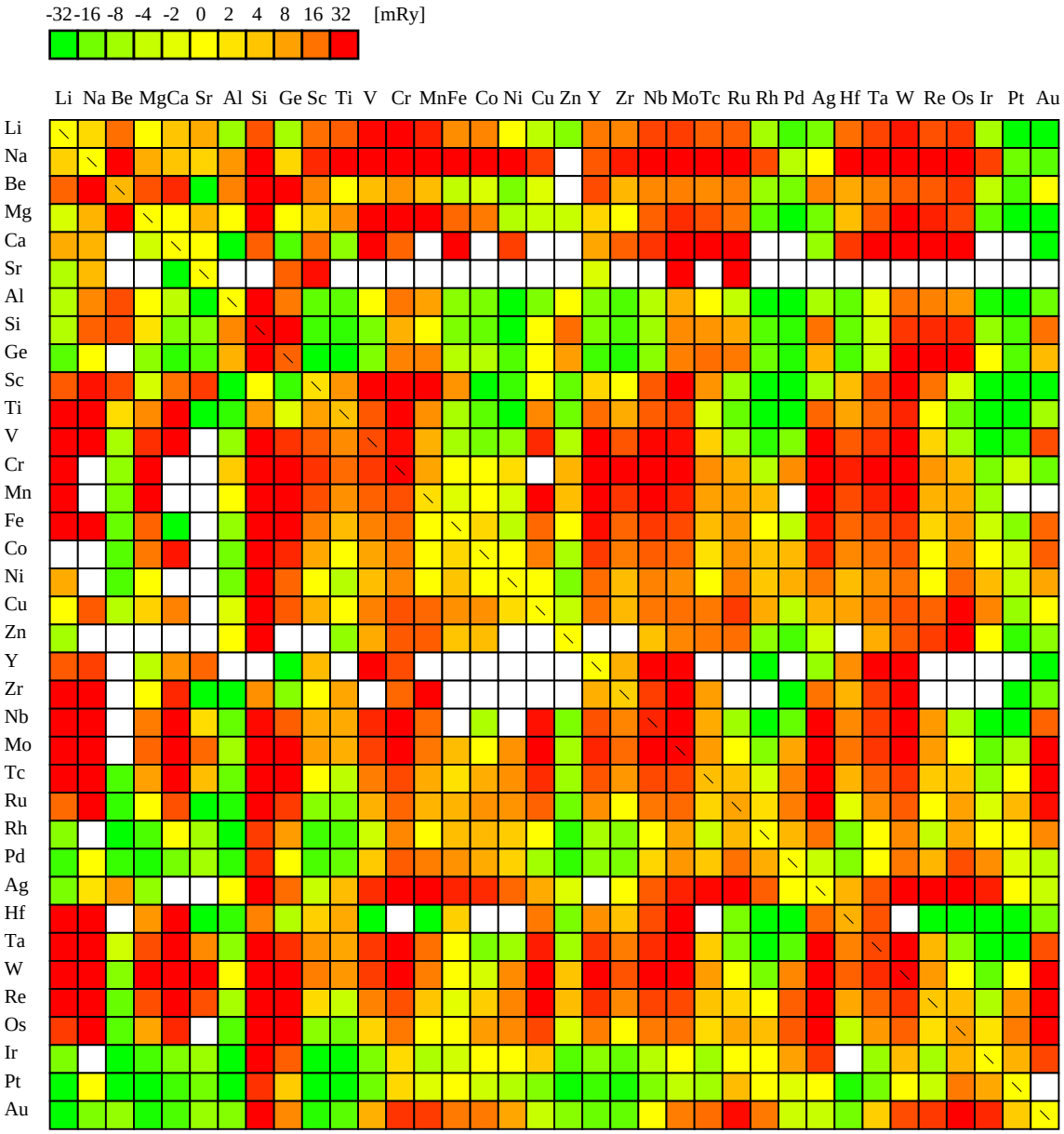
Formation energies for B2

Alloy: AB



Formation energies for L12

Alloy: AB3



Fhndlr: Program: EQOS, Version: HLS 25 Nov 2002 TM: 11:32
isno= 0 03-Dec-02

KGRN: Code=KKR-CPA-SCA Lmax=d Core=Soft-core-A BZ=hex NK= 576
Job=TiHf30_A3-63 isno= 0 AFM=P XC=Perdew-Wang-96-LDA Struc=A3-63
it mmt nta Atom Conc(it,ita):
1 2 2 Ti 0.7000 Hf 0.3000

Ground state parameters: LDA

Sws_eq =	3.060358 Bohr;	Vol =	120.06 Bohr**3
Sws_exp=	3.053300 Bohr;	Rho =	8.12 g/cm3
E_eq =	-10246.146432 Ry/atom;	E_form =	0.005563 Ry/atom
Bmod =	1.268996 Mbar;	Bmod =	126.90 GPa
dB/dP =	7.119843	Gamma =	3.0599
Error =	0.000215 Ry(rms);	Alpha =	21.06E-6 at 300.K

Ground state parameters: GGA

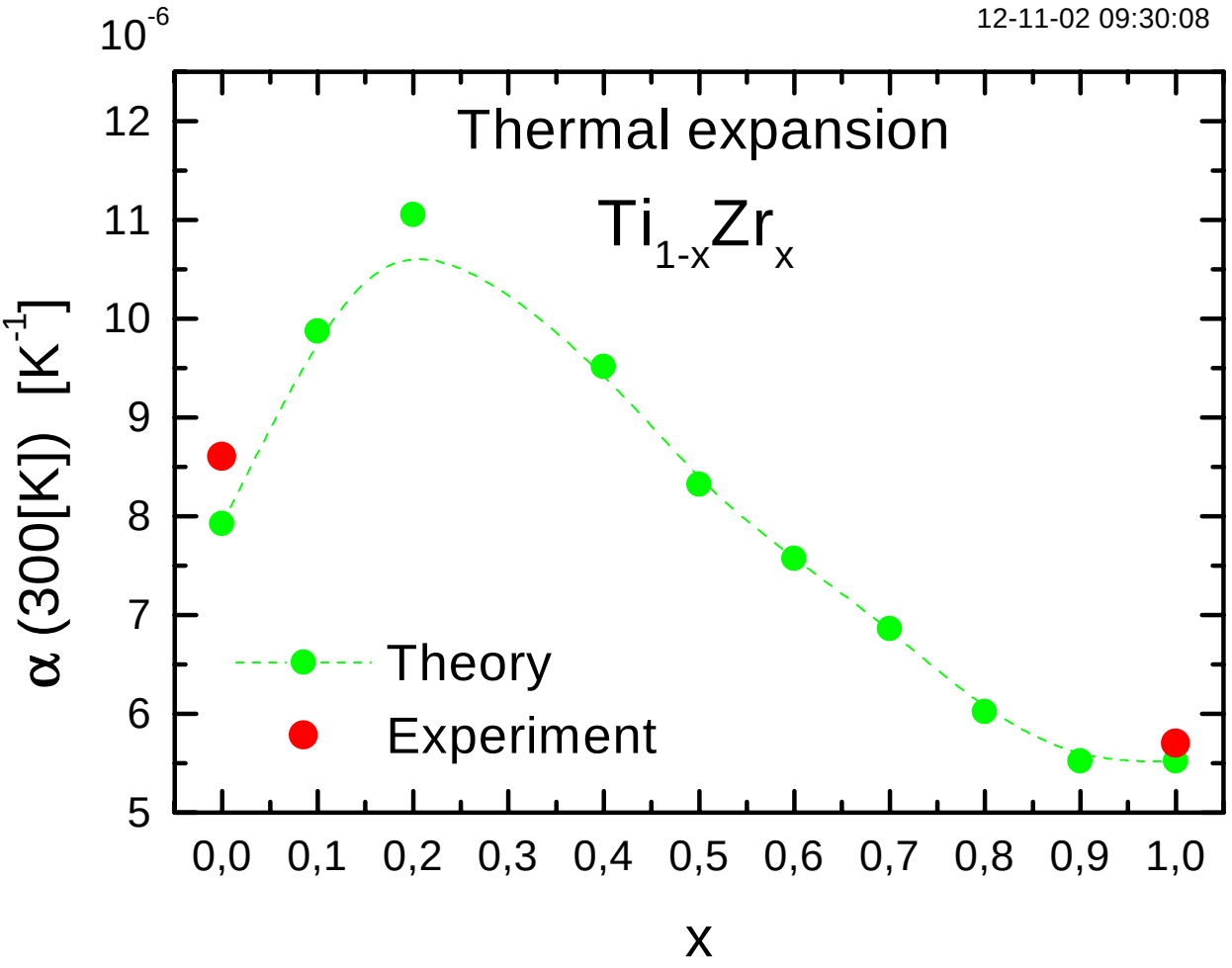
Sws_eq =	3.148182 Bohr;	Vol =	130.70 Bohr**3
Sws_exp=	3.053300 Bohr;	Rho =	7.46 g/cm3
E_eq =	-10254.081756 Ry/atom;	E_form =	0.006196 Ry/atom
Bmod =	0.838916 Mbar;	Bmod =	83.89 GPa
dB/dP =	6.580839	Gamma =	2.7904
Error =	0.000231 Ry(rms);	Alpha =	27.18E-6 at 300.K

Ground state parameters: LAG

Sws_eq =	3.105742 Bohr;	Vol =	125.48 Bohr**3
Sws_exp=	3.053300 Bohr;	Rho =	7.77 g/cm3
E_eq =	-10247.706519 Ry/atom;	E_form =	0.005799 Ry/atom
Bmod =	1.007090 Mbar;	Bmod =	100.71 GPa
dB/dP =	6.681897	Gamma =	2.8409
Error =	0.000213 Ry(rms);	Alpha =	23.70E-6 at 300.K

Eqos: The formation energies [Ry/atom]

S[au]	LDA	GGA	LAG
2.916300	0.019914	0.035853	0.027310
2.966300	0.010592	0.021960	0.015772
3.016300	0.006908	0.014101	0.009894
3.066300	0.005738	0.009024	0.006632
3.116300	0.006837	0.006433	0.005724
3.166300	0.009953	0.006083	0.006918
3.216300	0.014863	0.007741	0.009995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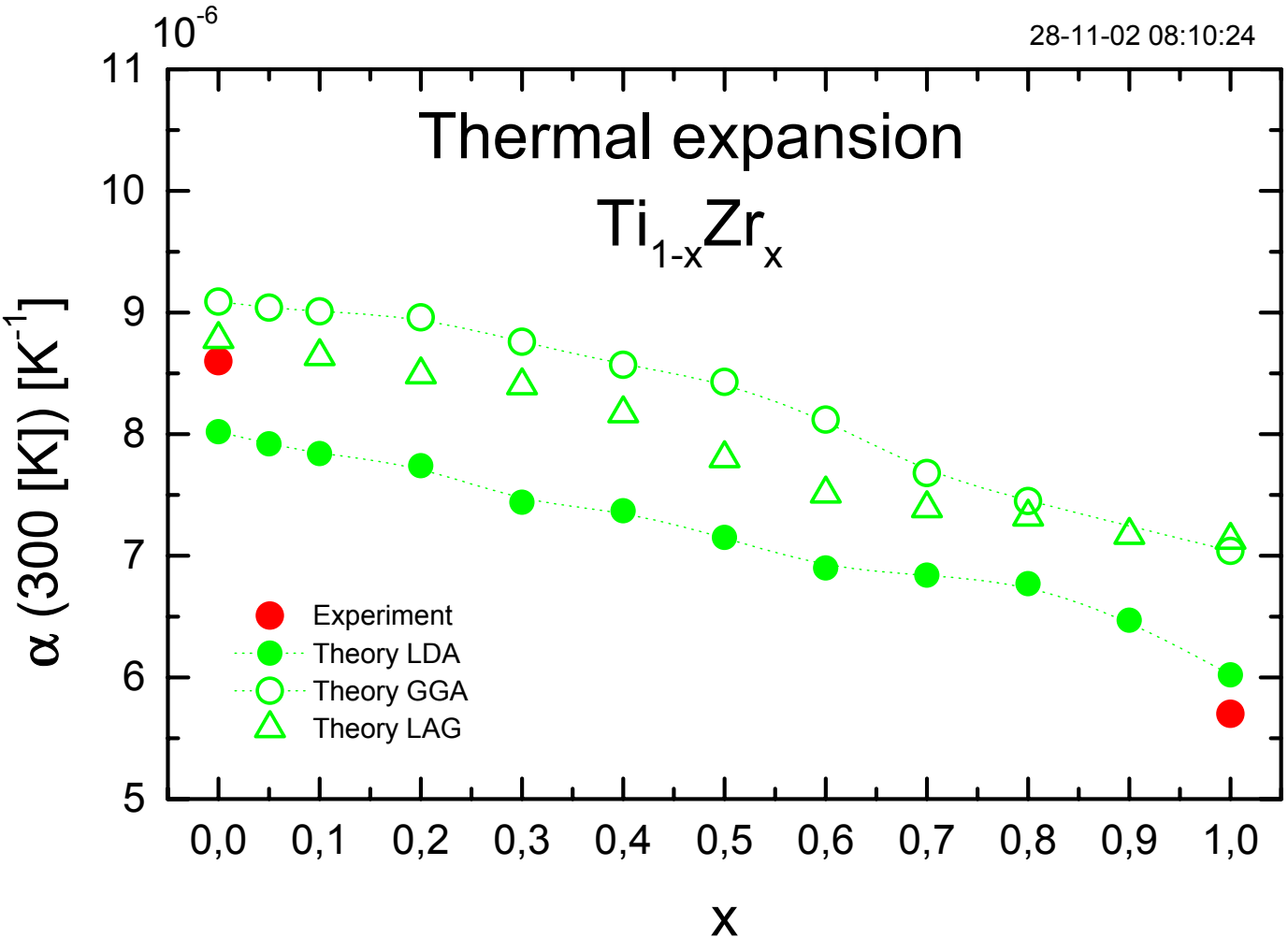
Thermal expansion
Ti1-xZrx
10-6
α (300[K]) [K-1]
12
11
10
9
8
7
6
5
0,0
0,1
0,2
0,3
0,4
0,5
0,6
0,7
0,8
0,9
1,0
x
Theory
Experiment


28-11-02 08:10:24
Thermal expansion
Ti1-xZrx
10-6
α (300 [K]) [K-1]
11
10
9
8
7
6
5
0,0
0,1
0,2
0,3
0,4
0,5
0,6
0,7
0,8
0,9
1,0
x
Experiment
Theory LDA
Theory GGA
Theory LAG

NIFLHEIM

The 2-TeraFLOPS cluster supercomputer

The NIFLHEIM cluster supercomputer was installed on August 12, 2002 at Center for Atomic-scale Materials Physics (CAMP) at the Technical University of Denmark (DTU), with a grant from the Danish Center for Scientific Computing (DCSC).
This resource is available only to grant holders within DCSC.
Consisting of 480 PCs, the cluster's total peak performance is above 2.1 TeraFLOPS (2.1 million million floating-point operations per second). This makes it one of the fastest computers in Europe at the time of installation.
A sister installation under DCSC is the Horseshoe cluster at the University of Southern Denmark. The two clusters were planned together and consist of grand total of 1000 PCs from Compaq.

Further information about NIFLHEIM:

NIFLHEIM

The name

The NIFLHEIM cluster supercomputer was given a name through a naming competition held at CAMP in the summer of 2002.

In Nordic mythology, Niflheim is the land of fog and ice, and Niflheim is part of the myth of creation: When the heat from Muspelheim melted the first drops of water from the ice of Niflheim, these drops formed into the giant Ymer, the first living creature. When Ymer was later killed, his dead body was molded into the world as we know it.

Read more about the Edda prose containing the Nordic myth of creation in this translation into English (check out Chapter 4, *The Creation Of The World*).

The NIFLHEIM cluster supercomputer is actually housed in a basement room with chilled air cooling, and NIFLHEIM is thus bitterly cold. This room is officially known as the *Fog Room* (in Danish: *Tågerummet*) because it was originally built with the purpose of experiments in the mid-1960'ies by Prof. R. E. H. Rasmussen trying to precipitate fog using electrical fields.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