Bond Order Potentials for AlCuH and C

available from LAMMPS site or us

2015 LAMMPS Users' Workshop and Symposium

UNM Continuing Education Building, NM, August 5-7, 2015

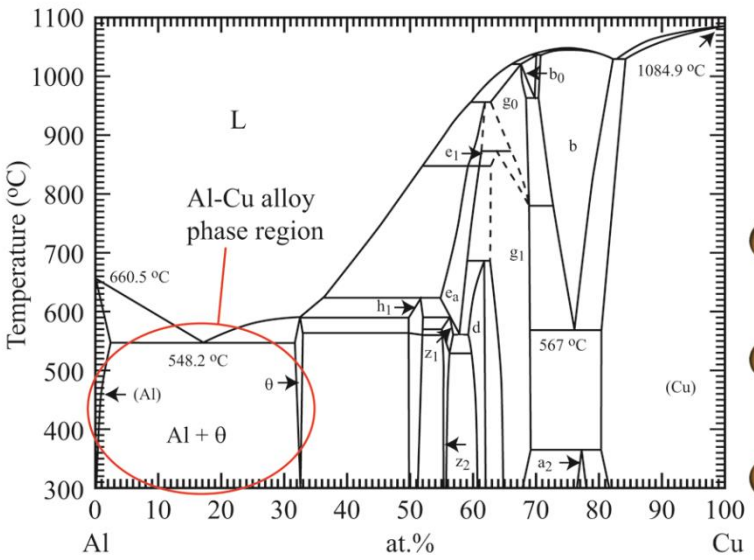
X. W. Zhou, D. K. Ward, M. E. Foster, and J. A. Zimmerman
Sandia National Laboratories, USA

This work is supported by a Laboratory Directed Research and Development (LDRD) project. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

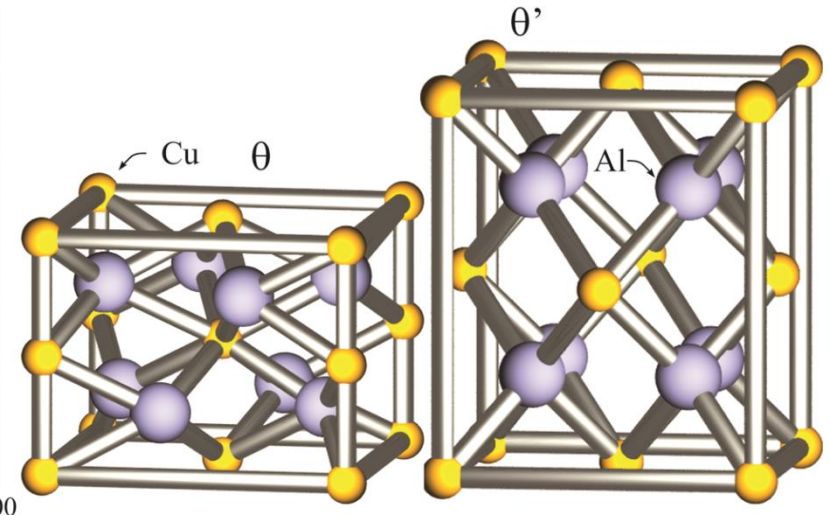
Wish List for AlCuH Potential

1. A high stacking fault energy of Al observed in experiments;
2. Properties trends of a variety of stable and metastable structures;
3. Al-rich side of the Al-Cu phase diagram;
4. A reasonable positive heat of solution of Cu in Al;
5. H2 $\Leftrightarrow$ 2H chemical reaction;
6. $Al_{1-x}H_x \rightarrow Al + H_2$ and $Cu_{1-x}H_x \rightarrow Cu + H_2$ phase separations;
7. Robust MD simulations.

(a) Al-Cu phase diagram



(b) crystal structure of the θ and θ' phases



X. W. Zhou, D. K. Ward, and M. E. Foster, manuscript to be submitted, potential available upon request

Stacking Fault Energy of Al

Model/Exp.	γ_{100}	γ_{110}	γ_{111}	γ_{sf}
EAM-CY	583	631	526	1
EAM-Mishin1	947	1013	873	141
EAM-BAM	1017	1154	1003	85
EAM-VC	862	969	829	71
EAM-MSAH	194	328	138	126
EAM-Zhou	868	958	832	44
EAM-MKBA	495	582	427	125
EAM-JNP	977	1055	910	0
MEAM	903	944	599	141
REAX-LJGS	481	483	427	0
REAX- Ojwang	810	848	711	1
BOP	979	1069	850	133
DFT [38]	1063	1098	987	------
Exp. [59,60,61,62]	980-1140	980-1140	980-1140	120-144

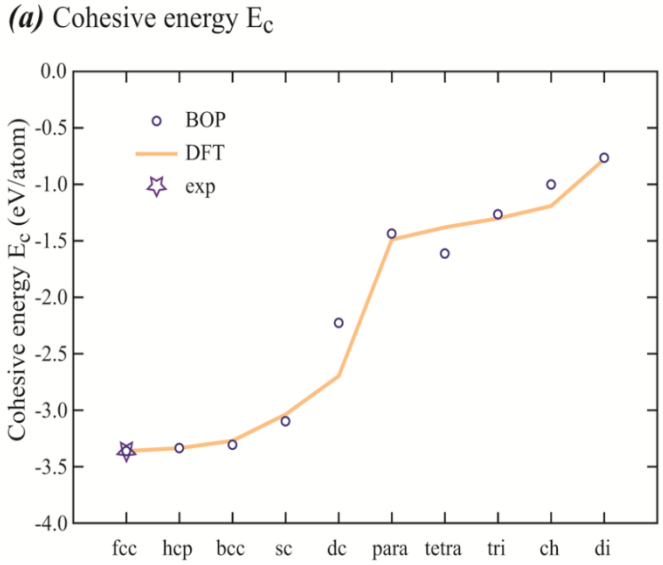
BOP captures a high stacking fault energy of Al.

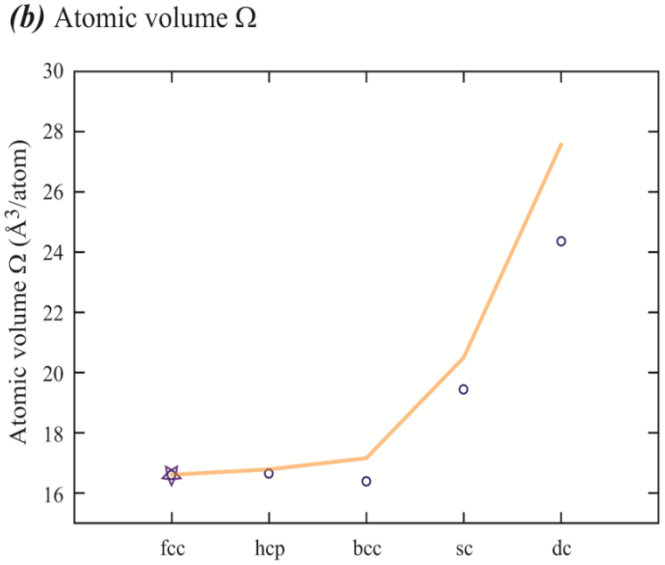
X. W. Zhou, D. K. Ward, and M. E. Foster, manuscript to be submitted, potential available upon request

Property Trends of Al and Cu

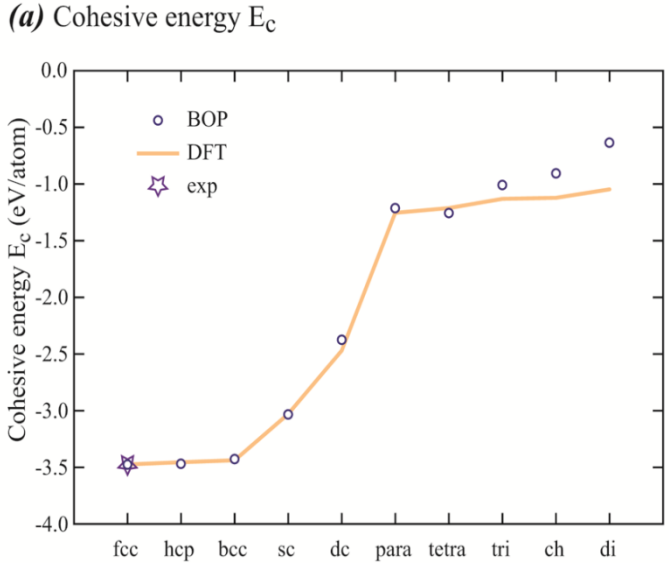
Sandia National Laboratories

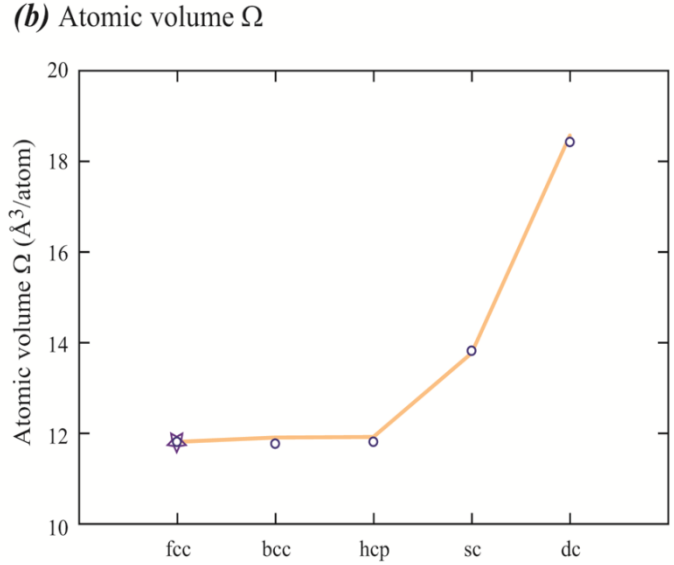
Al





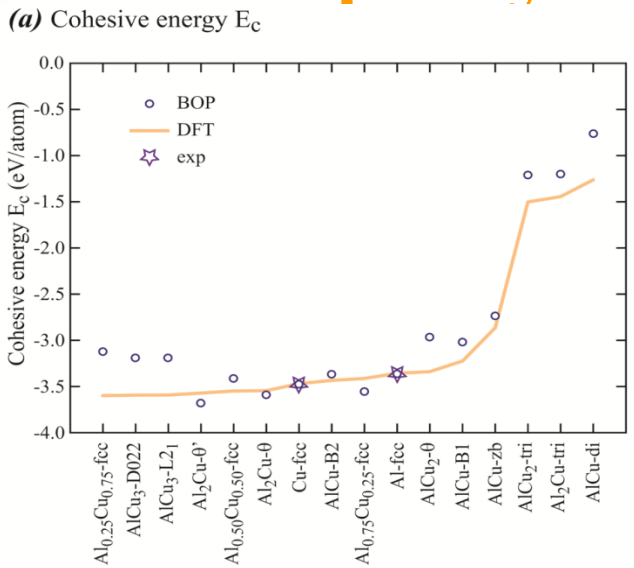
Cu

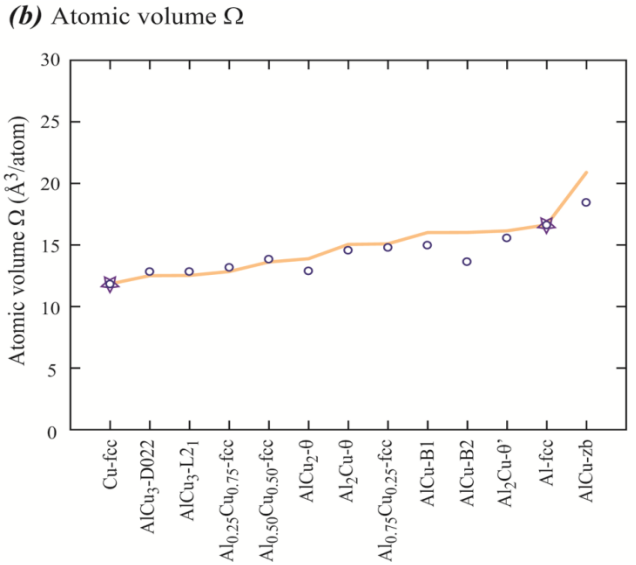




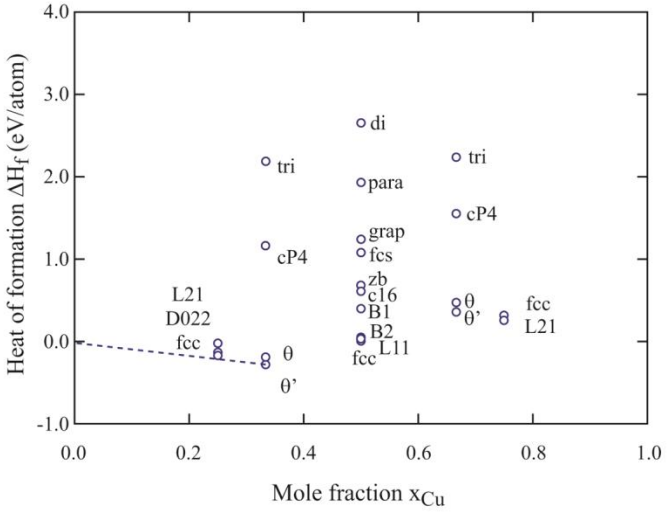
Pretty good property trends for Al and Cu.

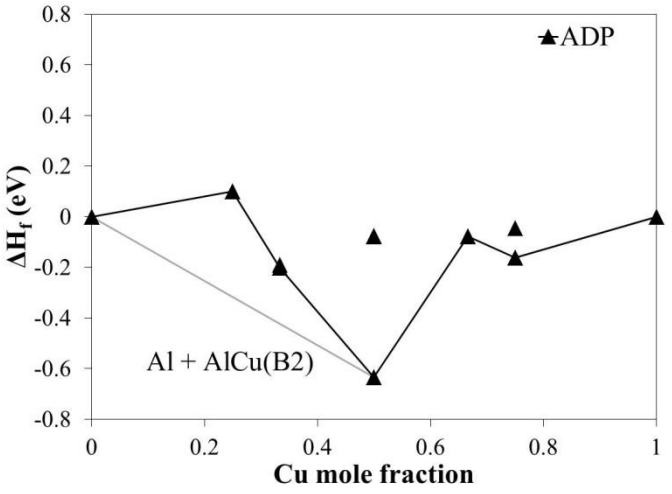
Property Trends of AlCu





Heat of Formation vs. Mole Fraction





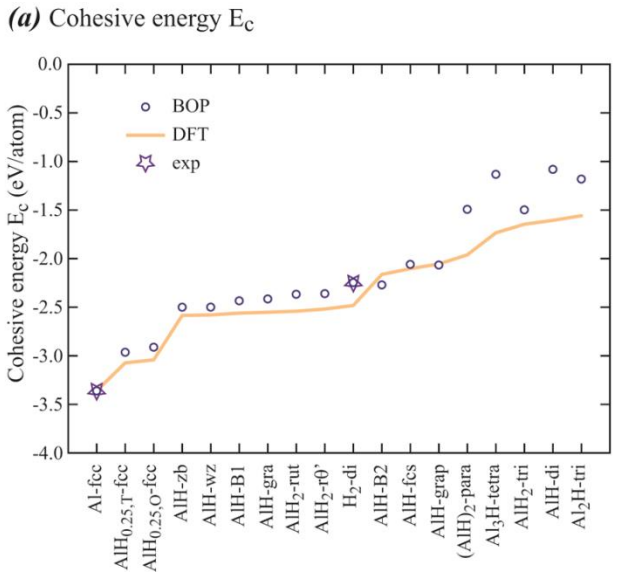
Pretty good property trends for AlCu.

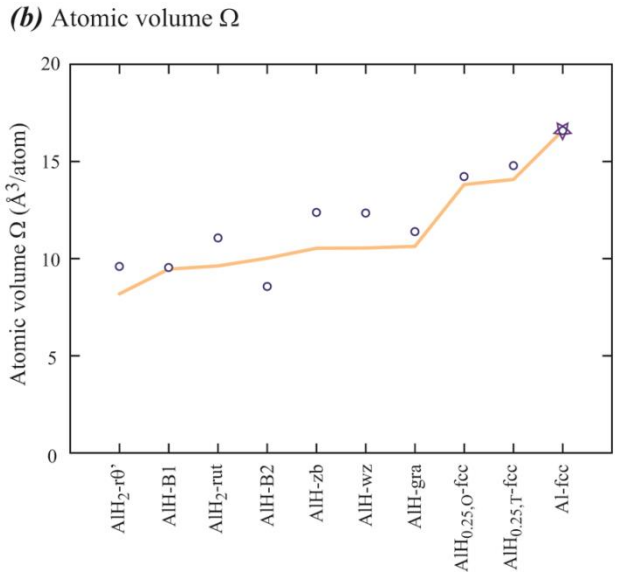
ADP: F. Apostol and Y. Mishin, Phys. Rev. B, 83, 054116 (2011).

Property Trends of AlH and CuH

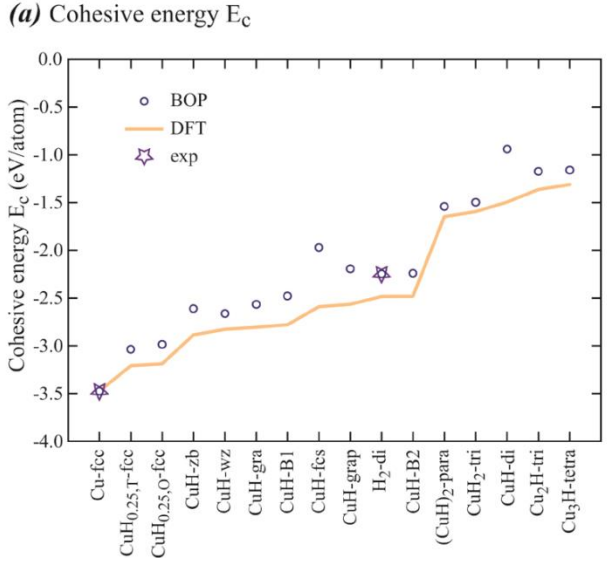
Sandia National Laboratories

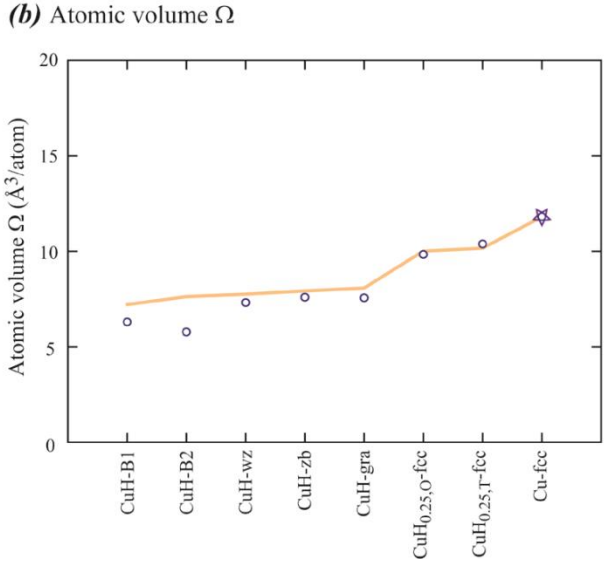
AlH





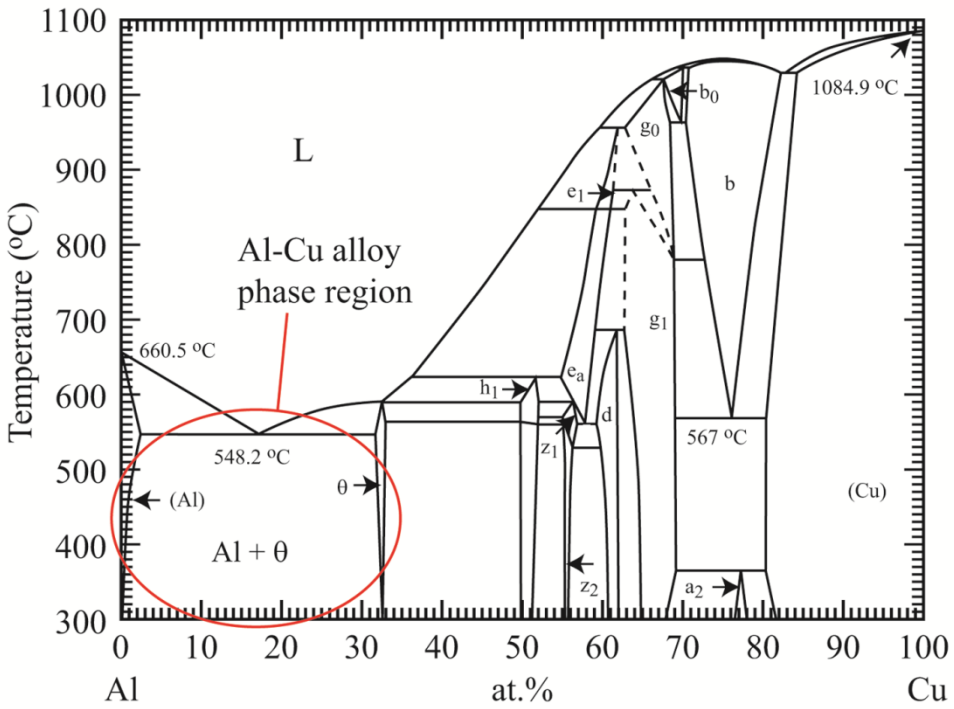
CuH

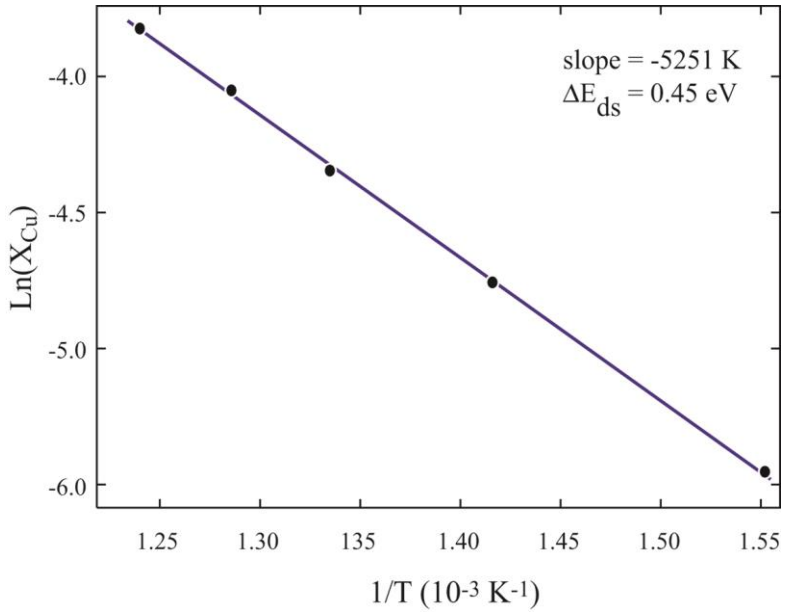




Pretty good property trends for AlH and CuH.

Dilute Heat of Solution of Cu in Al





1. Traditionally, heat of solution of Cu in Al is taken as energy change due to taking a Cu atom from Cu pool and putting it in Al pool;
2. Should really be the energy change due to taking a Cu atom from Al_2Cu pool and putting it in Al pool;
3. Must be a positive number

Results

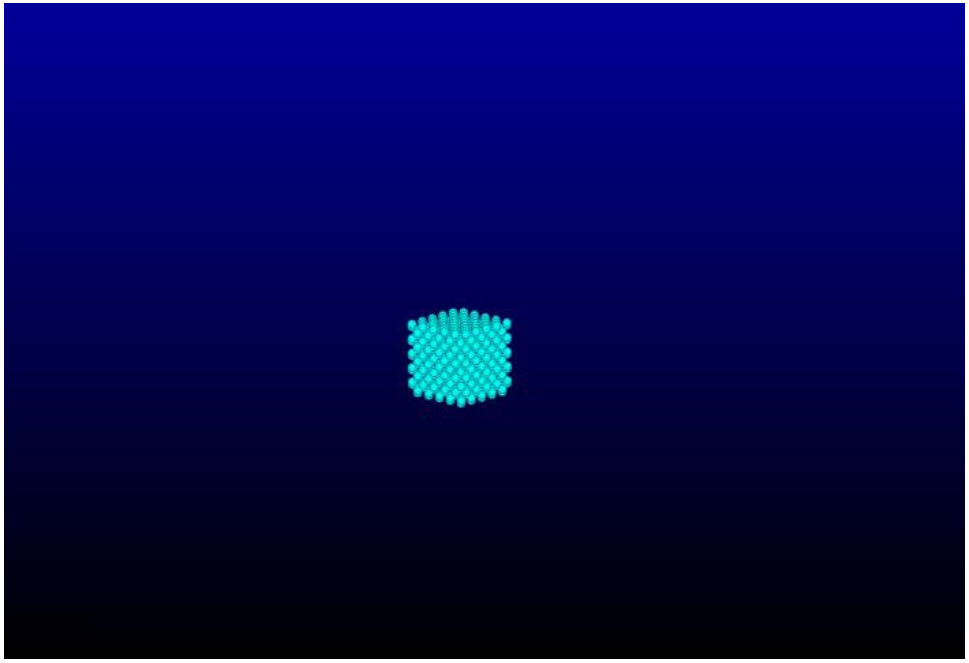
ADP	1.09
EAM-CY	-0.06
BOP	0.14
DFT	0.40
Exp.	0.45

X. W. Zhou, D. K. Ward, and M. E. Foster, manuscript to be submitted, potential available upon request

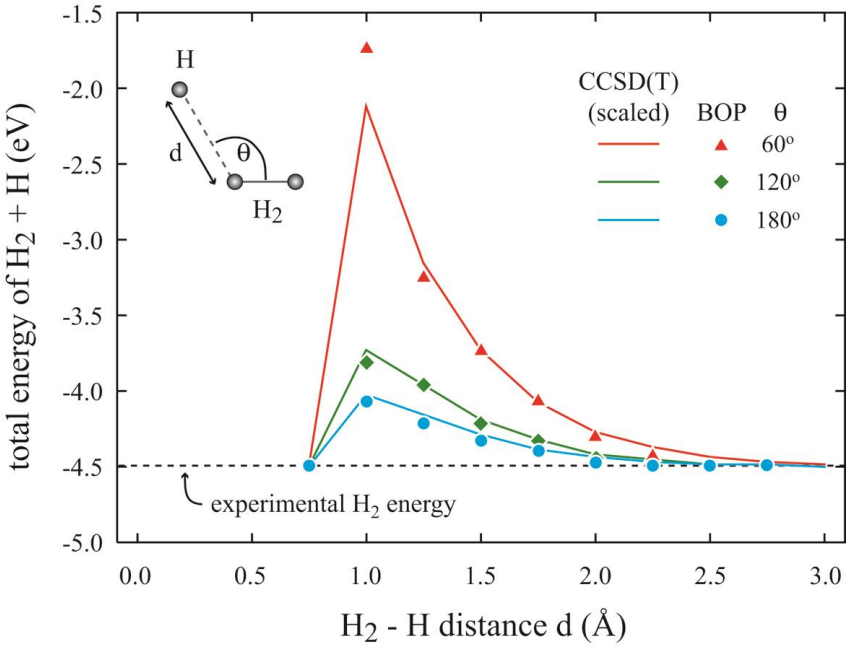
$H_2+H \rightarrow H+H_2$ Chemical Reaction

Sandia National Laboratories

Hydrogen crystal to H_2 gas



$H_2+H \rightarrow H+H_2$ energy profiles

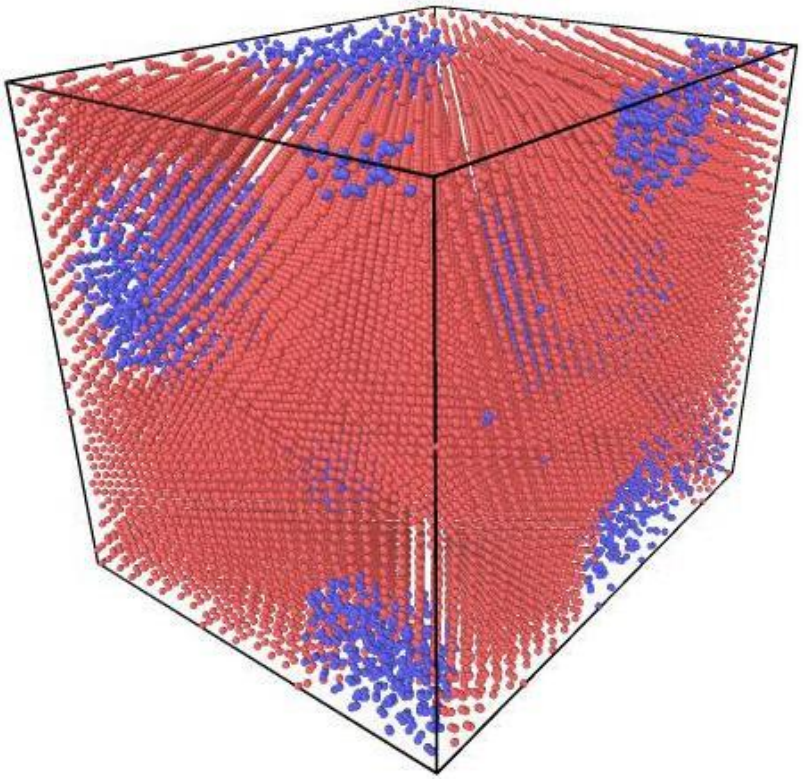


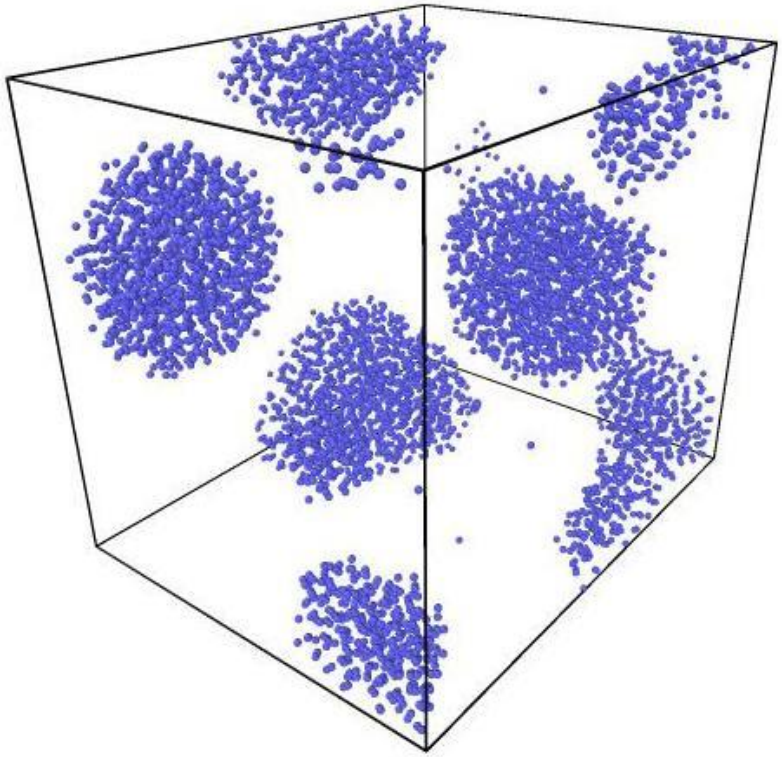
The BOP we developed has captured the $H_2+H \rightarrow H+H_2$ reaction, paper has been published: X. W. Zhou, D. K. Ward, M. Foster, J. A. Zimmerman, J. Mater. Sci., 50, 2859 (2015).

Al + H_2 and Cu + H_2 Phase Separation

(a) N_H/N_{Cu} = 0.20 with both Cu and H shown

(b) Only H shown



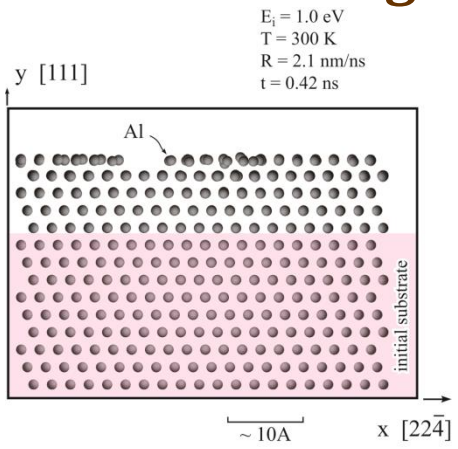


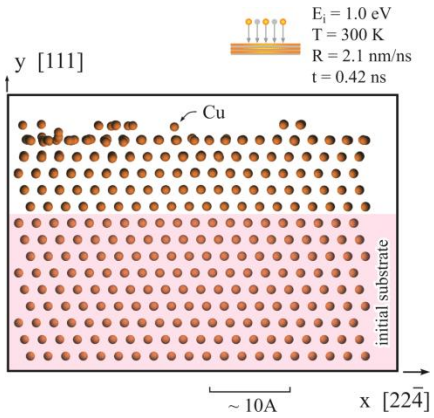
Phase separation is less pronounced in Al-H (see next slide), but Al forms AlH_3 compound.

Robust MD Simulations

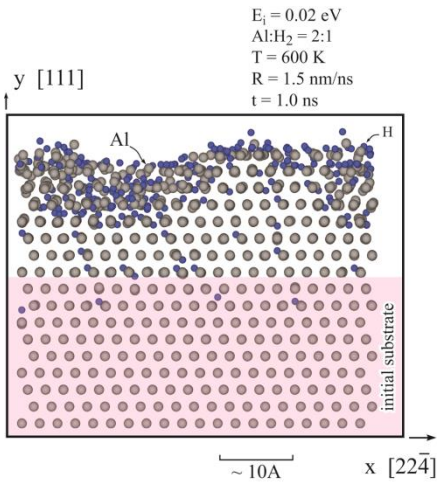
Sandia National Laboratories

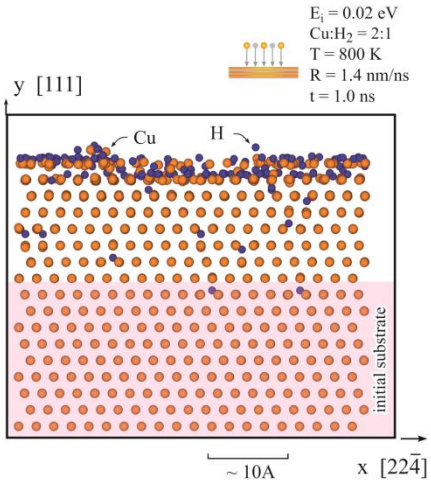
Al and Cu growth without H



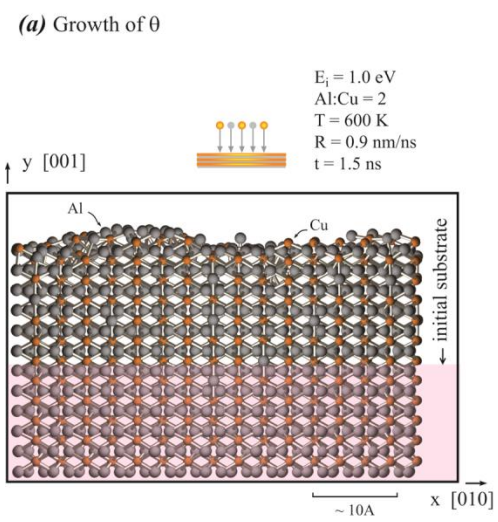


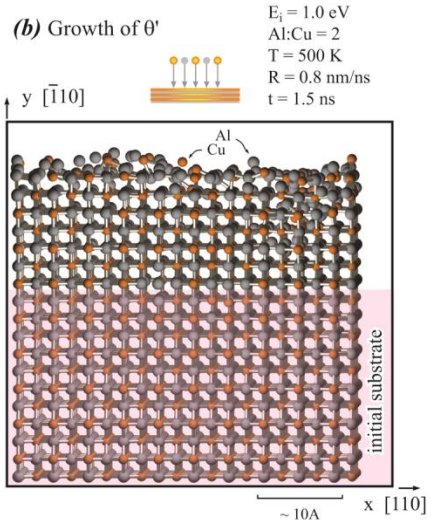
Al and Cu growth with H



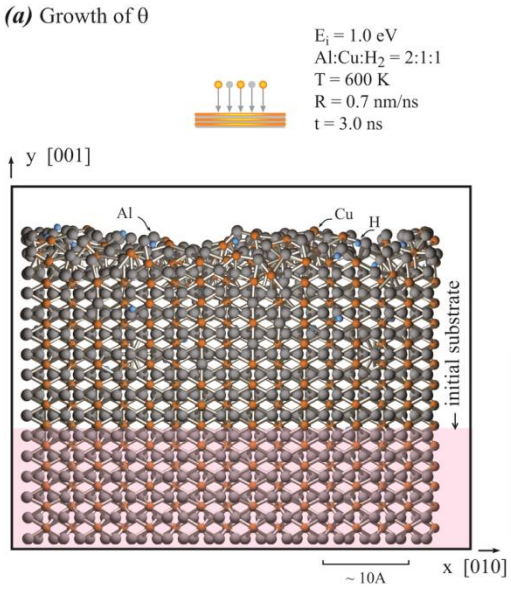


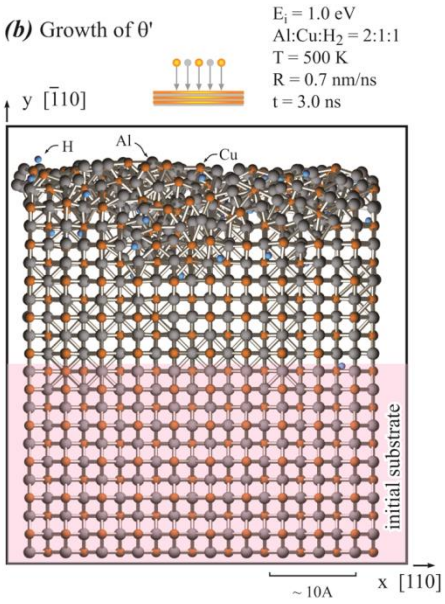
Al_2Cu (θ and θ') growth without H





Al_2Cu (θ and θ') growth with H





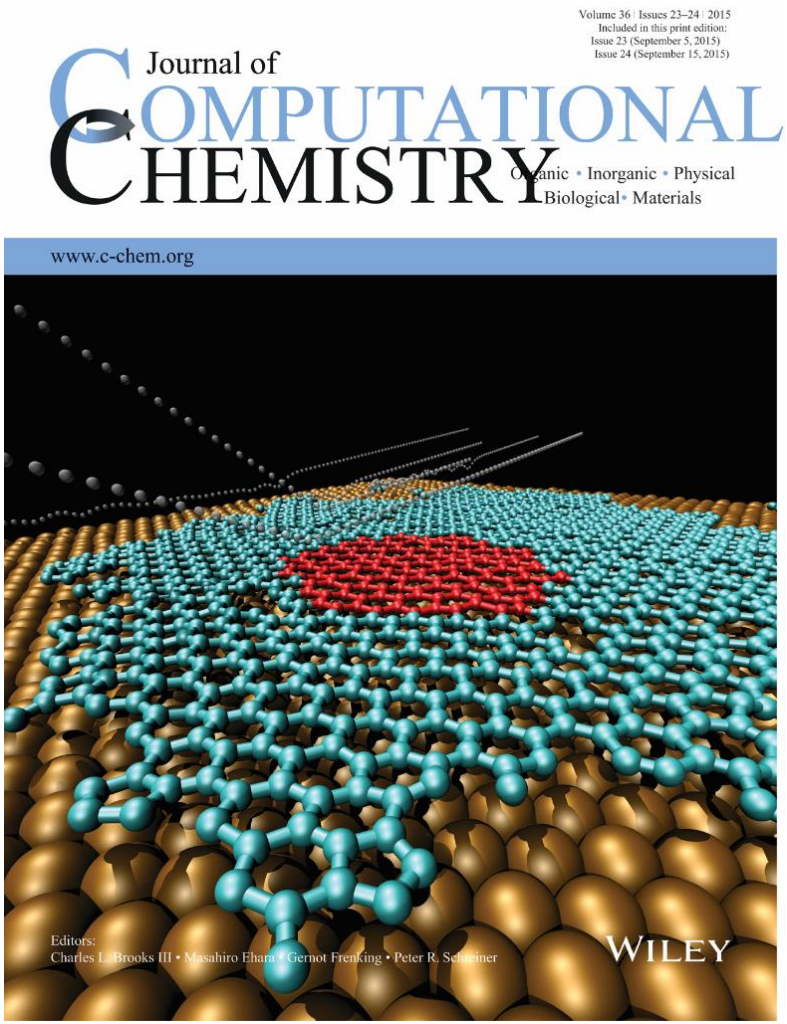
Dream Wish for C Potential

1. Direct MD simulation of graphene;
2. Energy transferability between graphene, graphite, diamond;
3. Robust MD simulations.

Our goal is to complement the existing C potentials:

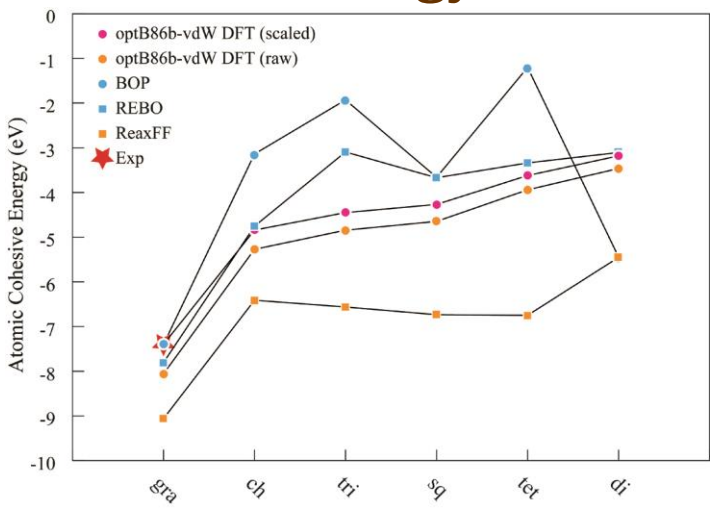
1. D. W. Brenner, O. A. Shenderova, J. A. Harrison, S. J. Stuart, B. Ni, and S. B. Sinnott, J. Phys.: Condens. Matter, 14, 783 (2002);
2. N. A. Marks, Phys. Rev. B, 63, 035401 (2001);
3. A. C. T. van Duin, S. Dasgupta, F. Lorant, and W. A. Goddard III, J. Phys. Chem., 105, 9396 (2001).

X. W. Zhou, D. K. Ward, and M. E. Foster, page 1719.

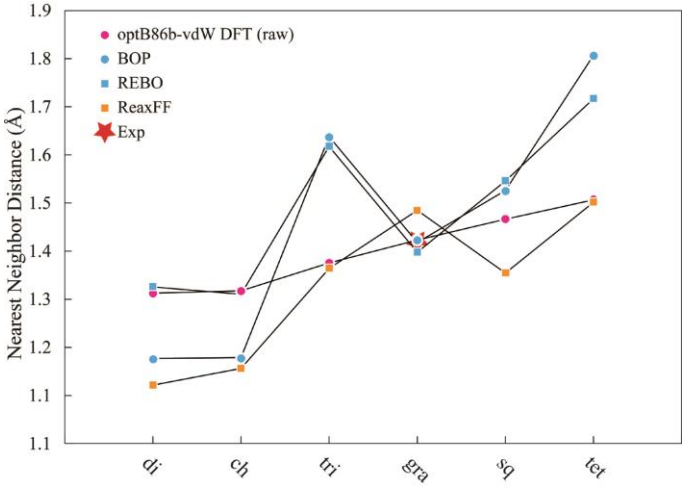


Property Trends

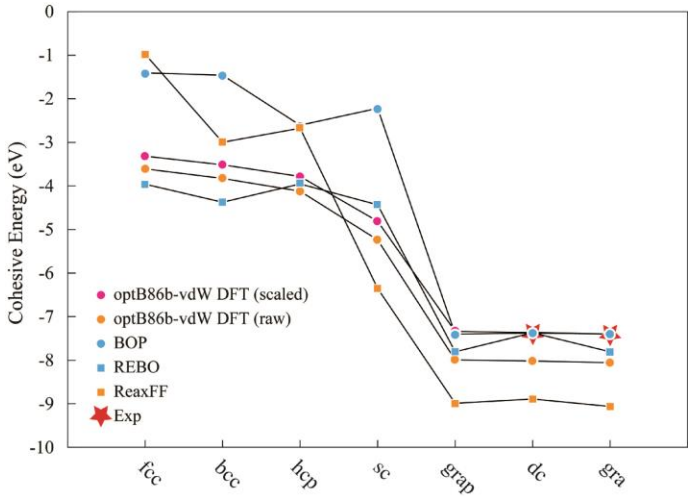
Cluster Energy Trends



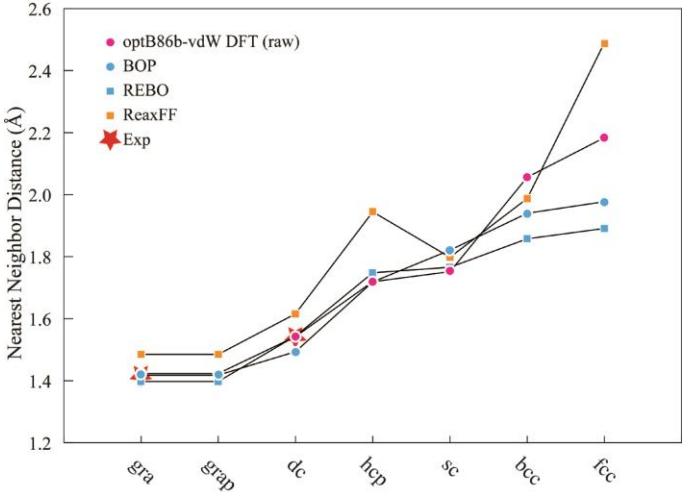
Cluster Size Trends



Lattice Energy Trends



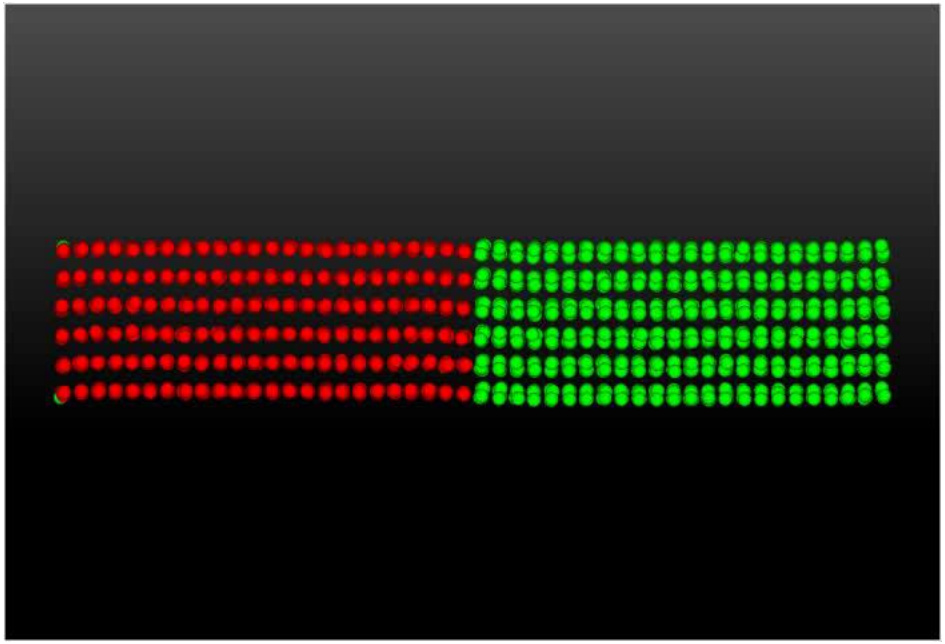
Lattice Size Trends



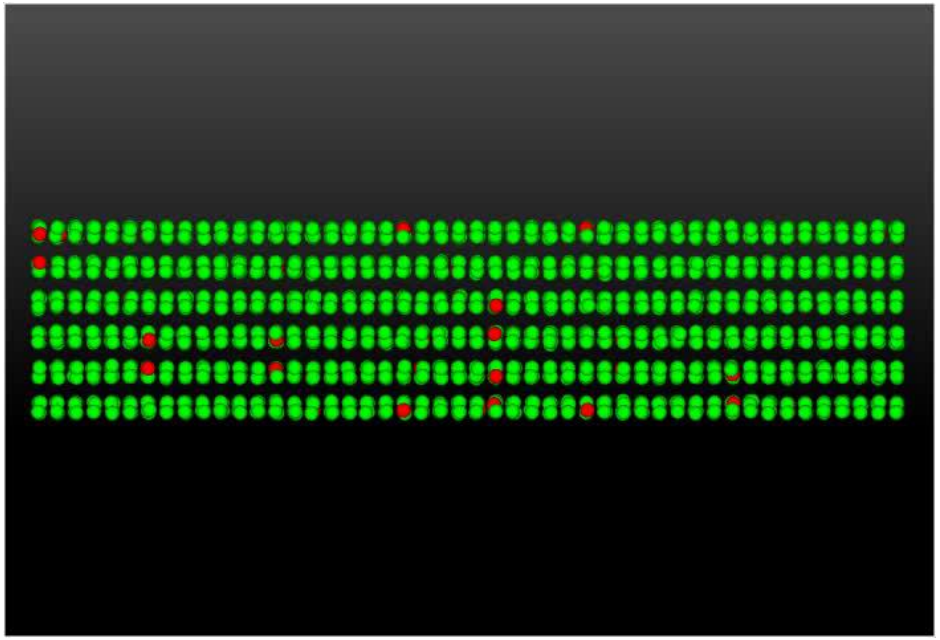
Robust MD Simulations

Graphite ⇔ Diamond Transformation

T = 2000 K, P = 0.6 Mbars

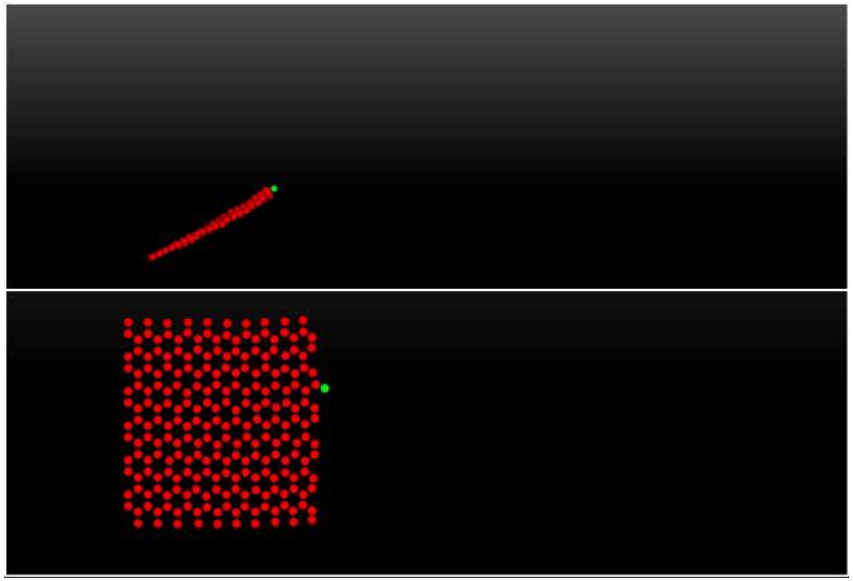


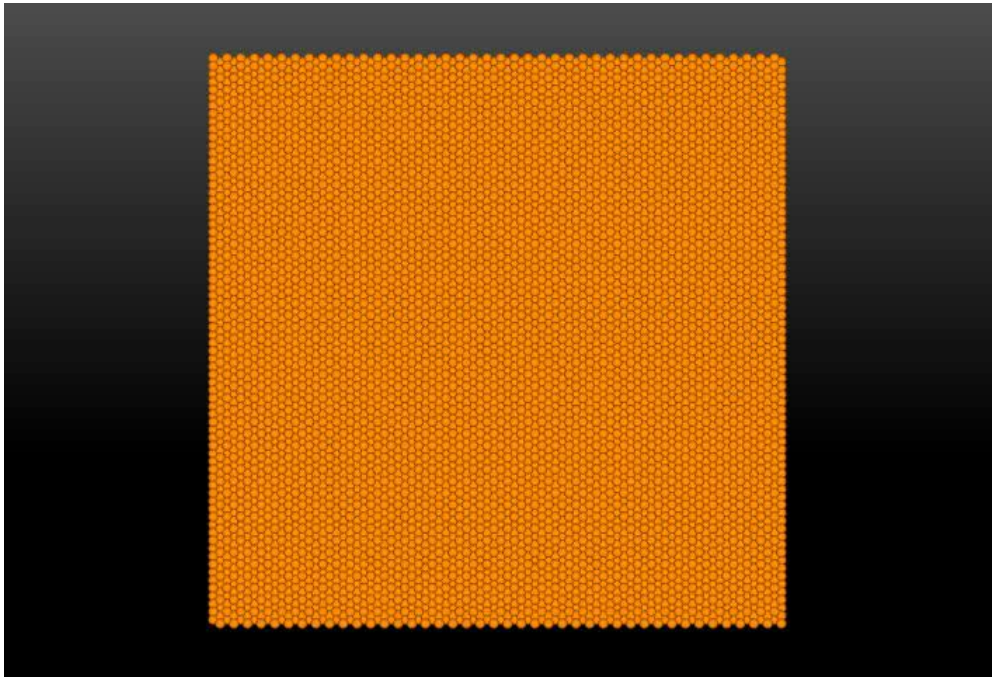
T = 1600 K, P = -0.6 Mbars (tensile)



Robust MD Simulations:

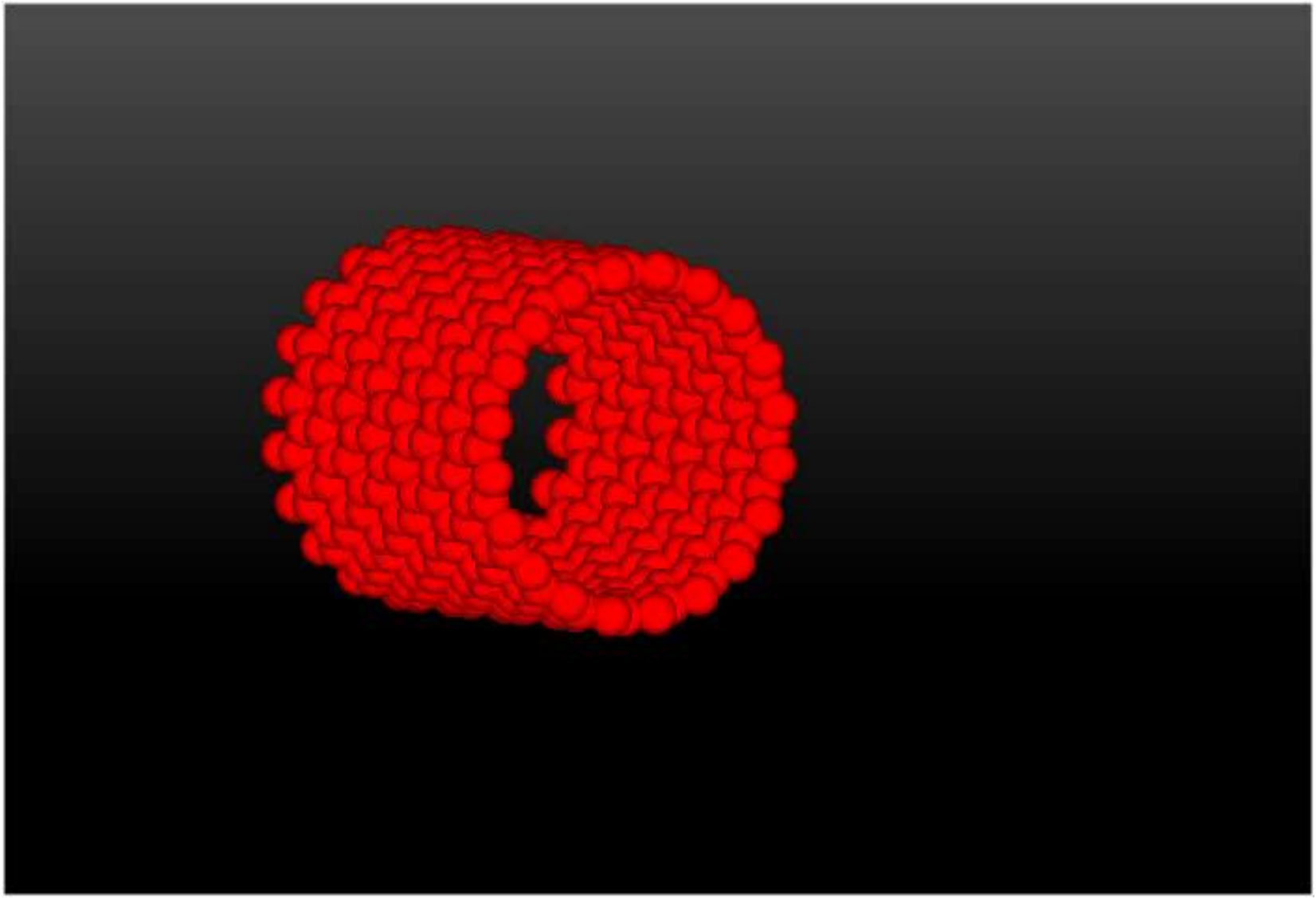
Graphene Growth





Robust MD Simulations

Nanotube Growth



Conclusions

1. Two bop potentials, AlCuH.bop, and C.bop, have been released to lammps package;
2. The AlCuH.bop meets the six+ criteria needed to study mechanical properties of AlCu alloys;
3. C.bop enables MD simulation of graphene growth.