Development of an Analytical Bond Order Potential for Al-Cu-H Systems

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Motivation: Aging of Al Alloys with H

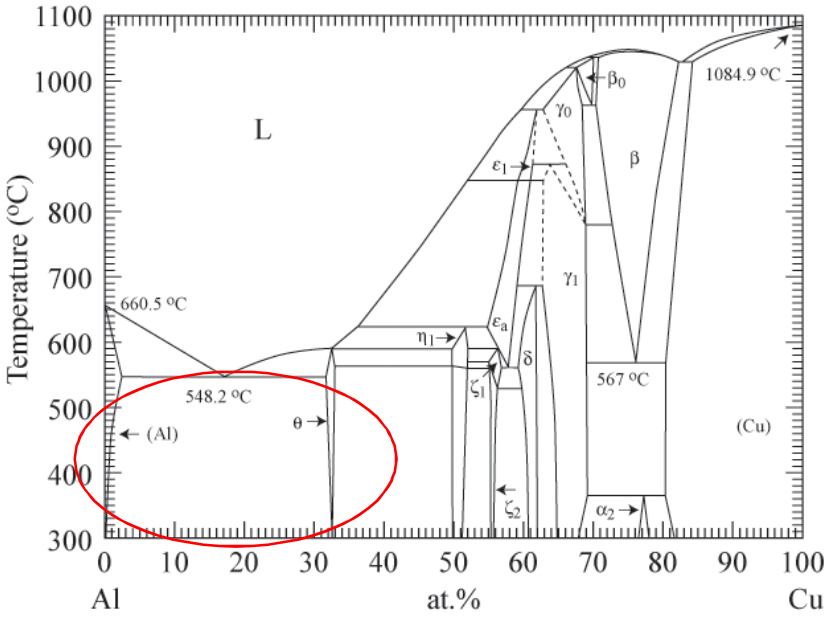
Al Alloys Promising for H-storage

Aluminum alloys: high strength-weight ratio, good thermal and electrical conductivities, low cost, high resistance to corrosion, and very low hydrogen solubility.

Issues: Long Time Aging Is Not Understood:

1. Long time interaction with hydrogen (e.g., adsorption, absorption, diffusion) is difficult to study with experiments alone.
2. Engineering scale continuum models for Al-H interaction require atomistic simulations to provide input.
3. To enable atomistic simulations, we develop an Al-Cu-H analytical bond order potential.

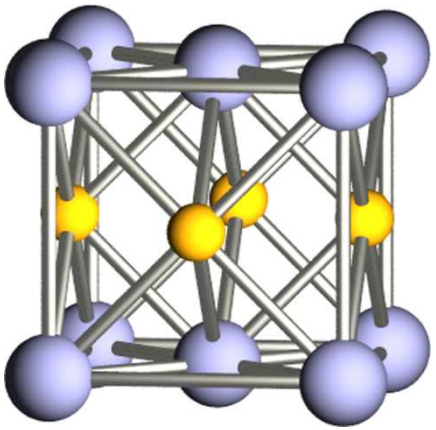
Extremely Challenging Atomistic Models



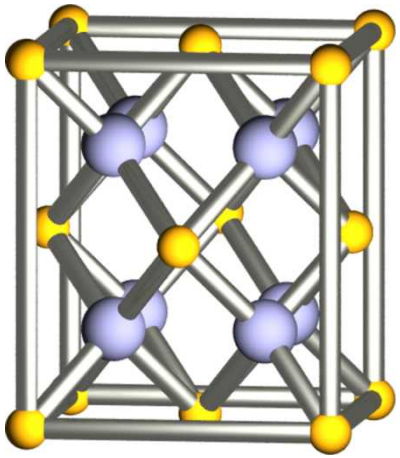
1. Model must incorporate various compound phases to predict the precipitate-strengthening effects.
2. Al_2Cu compounds (θ and θ') are the most important.
3. Precipitate formation: GP zone → θ' (CaF_2) → θ (Al_2Cu).

Can Model Even Captures These Crystals Structures?

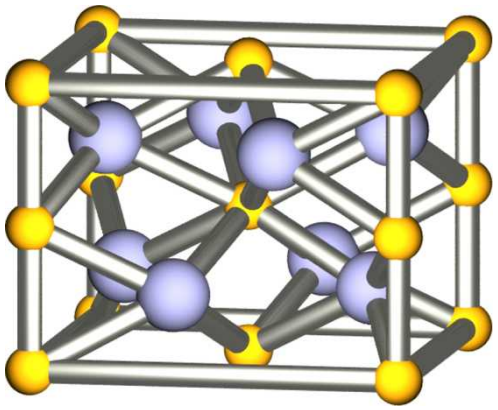
fcc (Al, Cu, GP zone)



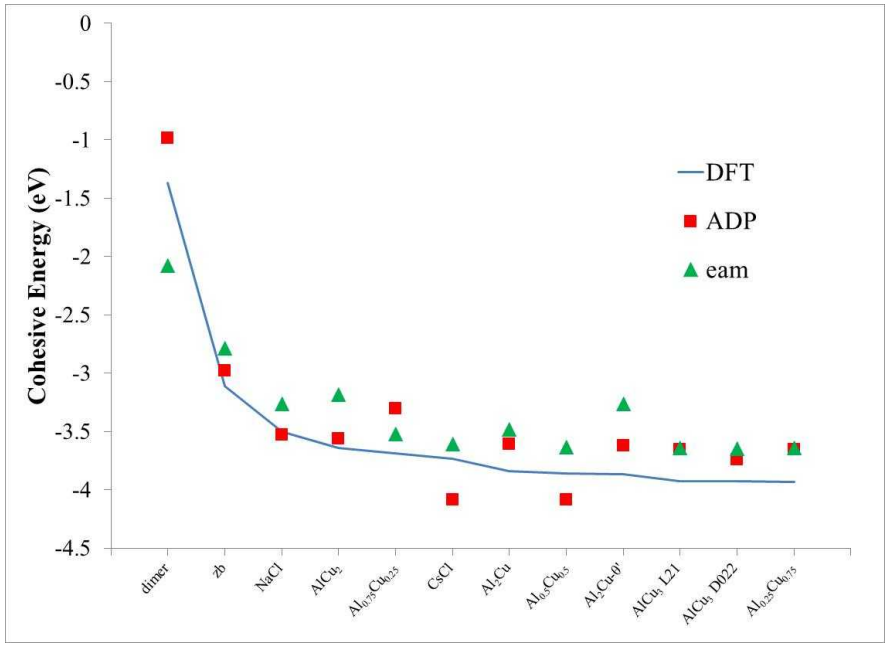
θ' (Al_2Cu)

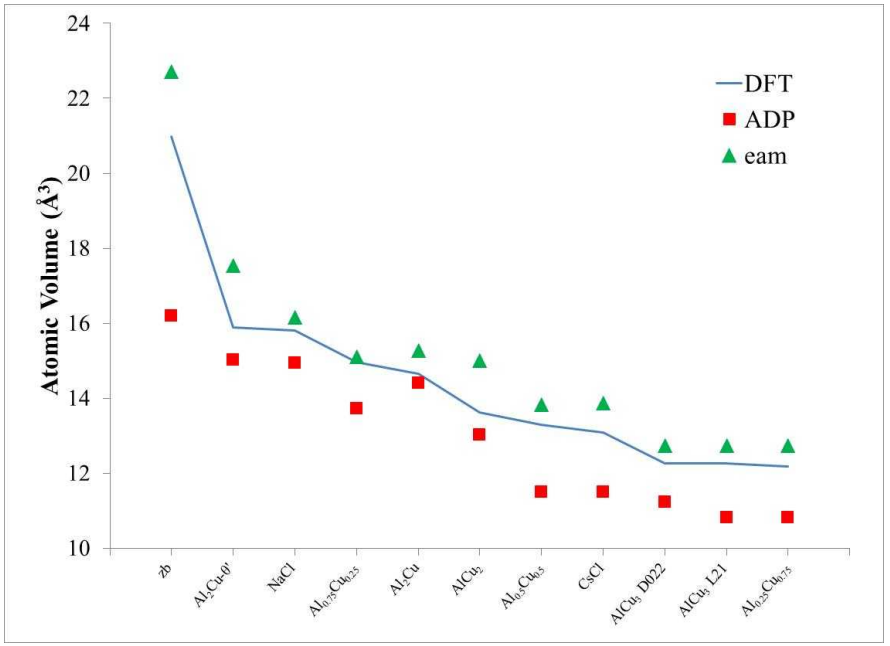


θ (Al_2Cu)



Property Trends of Different Literature Potentials



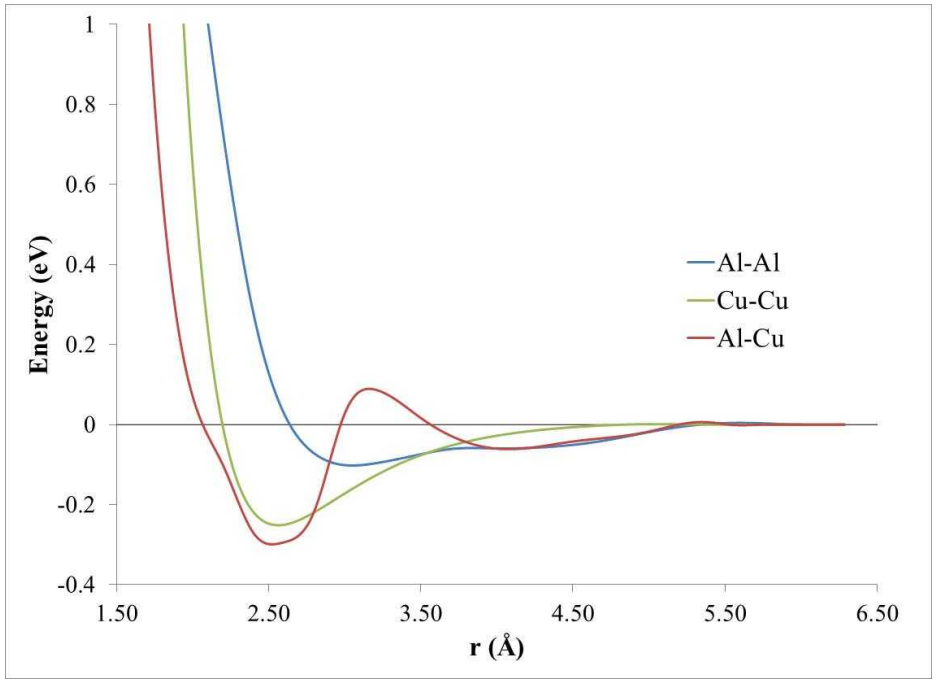


ADP: F. Apostol and Y. Mishin, PRB 83, 054116 (2011)
EAM: X.-Y. Liu et. al, Acta Mat. 47, 3227 (1999)

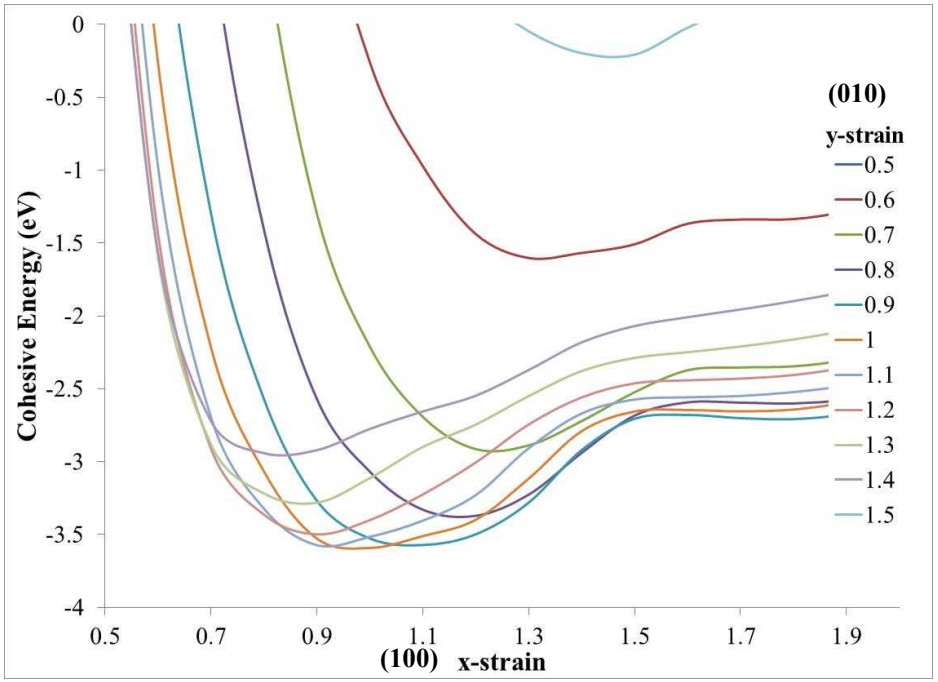
The Al-Cu potential developed by Mishin et al seems to be the best currently available.

Mishin Potential Observations I: Energy Wiggling

Pair potential functions

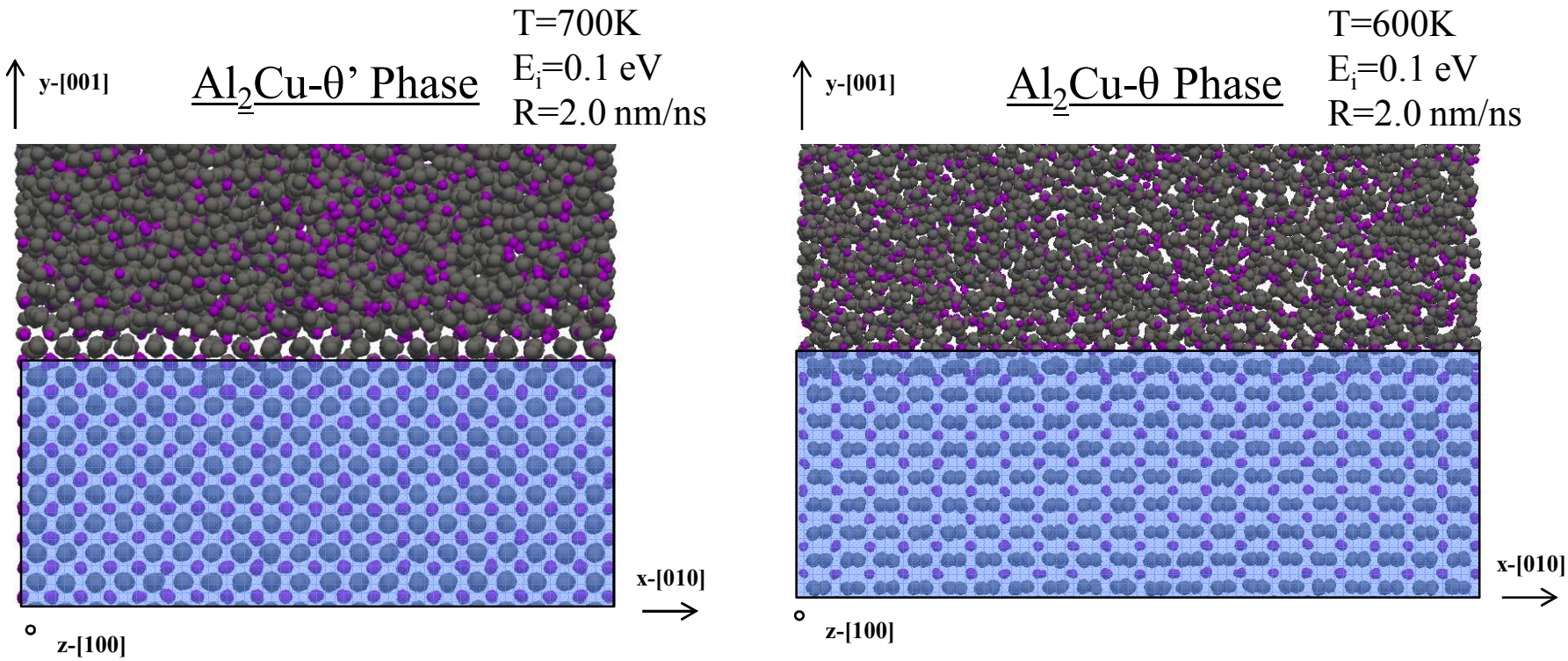


AlCu L_{21} structure



ADP: F. Apostol and Y. Mishin, PRB 83, 054116 (2011)

Mishin Potential Observations II: Growth Simulation of Al_2Cu Compounds



ADP: F. Apostol and Y. Mishin, PRB 83, 054116 (2011)

Growth Simulation Enabling Potentials

We aim to meet two criteria:

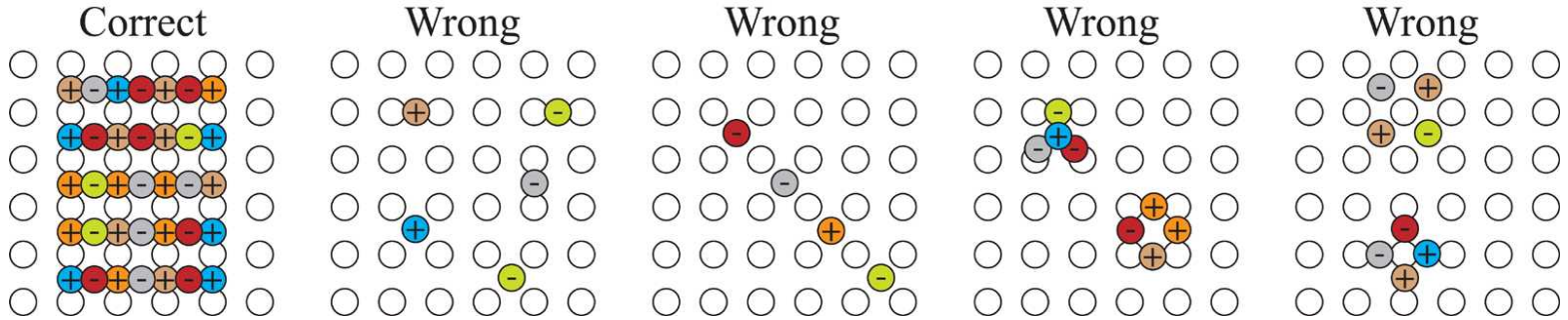
1. Captures property trends of many phases as determined from quantum calculations;
2. Predicts correctly crystalline growth during MD simulations.

Note that:

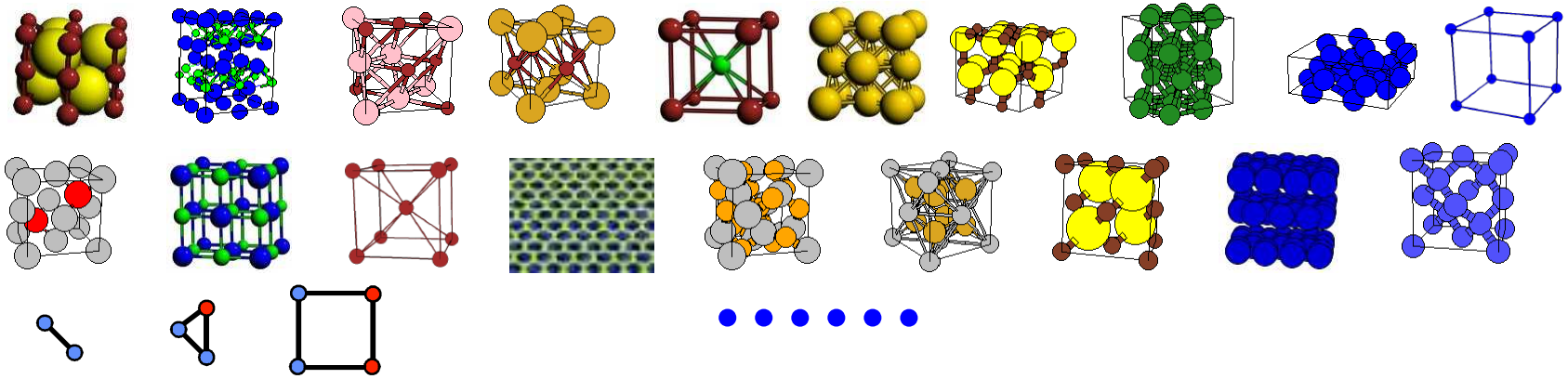
1. Growth simulations test unlimited number of configurations;
2. Interatomic potentials are usually not tested for growth simulations $\Rightarrow$ rare to satisfy both criteria.

[8]Growth Simulations Extremely Challenging

- **Wrong configurations should and will nucleate due to random condensation of adatoms, but they must all evolve to the correct crystal structure;**



- **Capturing property trends of a large number of clusters, lattices, and defects are necessary, but this alone will not ensure successful growth simulations.**



- **Extensive iterations are usually needed to develop an growth-enabling interatomic potential.**

Analytical Bond Order Potential (BOP)

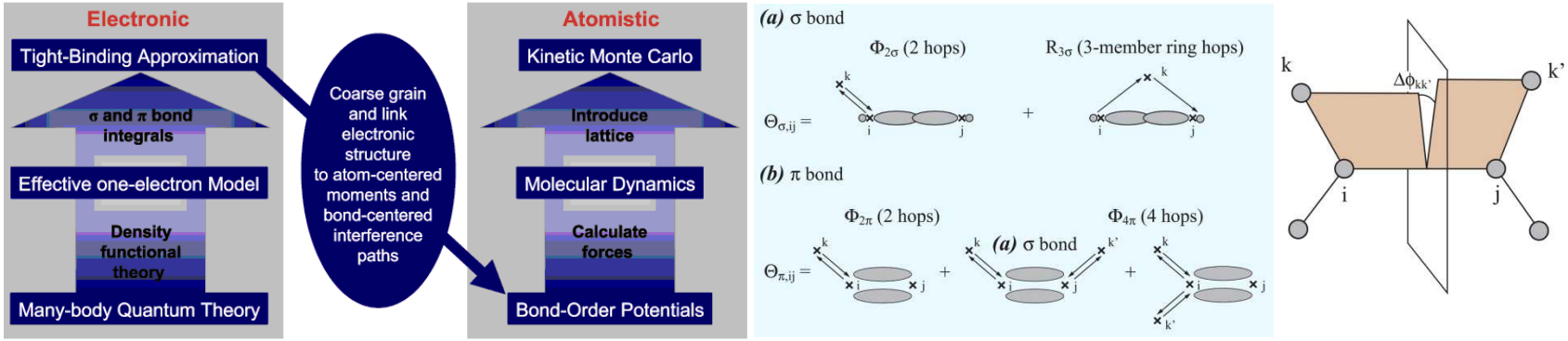
$$E = \frac{1}{2}\sum_i \sum_{j\neq i} \phi_{ij}(r_{ij}) - \sum_i \sum_{j\neq i} \beta_{\sigma,ij}(r_{ij}) \cdot \Theta_{\sigma,ij} - \sum_i \sum_{j\neq i} \beta_{\pi,ij}(r_{ij}) \cdot \Theta_{\pi,ij}$$

$\phi_{ij}(r_{ij})$: core-core repulsion; $\beta_{\sigma,ij}(r_{ij})$ and $\beta_{\pi,ij}(r_{ij})$: σ and π bond integrals describing electron hopping probabilities among different orbital's; $\Theta_{\sigma,ij}$ and $\Theta_{\pi,ij}$: σ and π bond orders describing half of difference in number of electrons in the bonding and anti-bonding states. $\Theta_{\sigma,ij}$ and $\Theta_{\pi,ij}$ are complicated functions of bond length and bond angles.

1. D. G. Pettifor, M. W. Finnis, D. Nguyen-Manh, D. A. Murdick, X. W. Zhou, and H. N. G. Wadley, Mater. Sci. Eng. A, 365, 2 (2004).
2. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. B, 59, 8487 (1999).
3. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. Lett., 84, 4124 (2000).
4. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. B, 65, 172103 (2002).
5. R. Drautz, D. Nguyen-Manh, D. A. Murdick, X. W. Zhou, H. N. G. Wadley, and D. G. Pettifor, TMS Lett., 1, 31 (2004).
6. R. Drautz, D. A. Murdick, D. Nguyen-Manh, X. W. Zhou, H. N. G. Wadley, and D. G. Pettifor, Phys. Rev. B, 72, 144105 (2005).
7. D. A. Murdick, X. W. Zhou, H. N. G. Wadley, D. Nguyen-Manh, R. Drautz, and D. G. Pettifor, Phys. Rev. B, 73, 45206 (2006).

Analytical Bond Order Potential

Cyrot-Lackmann theorem



1. **Derived from quantum mechanics theory through systematic coarse-graining;**
2. **Separate treatment of σ and π bonding energies** (products of bond order* and bond integral#);
3. **The first two levels of the expanded Green function retained for the σ and π bond orders;**
4. **Up to four electron hops are considered, naturally incorporating the 3-member ring term in the σ bonding ($R_{3\sigma}$) and the dihedral angle ($\Delta\phi_{kk'}$) effect in the p bonding;**
5. **Valence effect is addressed.**
6. **Accuracy comparable to quantum mechanics and scale comparable to conventional molecular dynamics.**

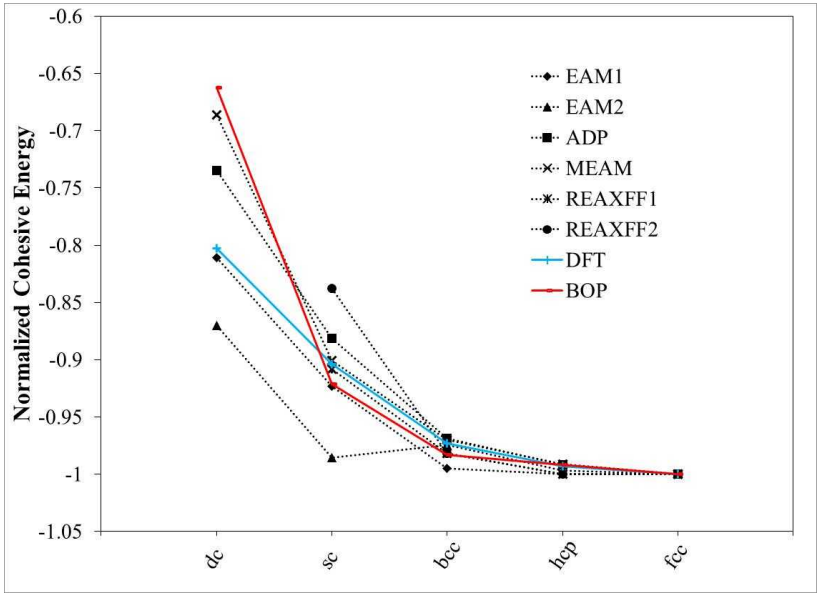
* bond order: half the difference of electrons in the bond and anti-boding states.
\# bond integral: hopping probability of electrons from one orbital to another.

BOP Parameterization Methods

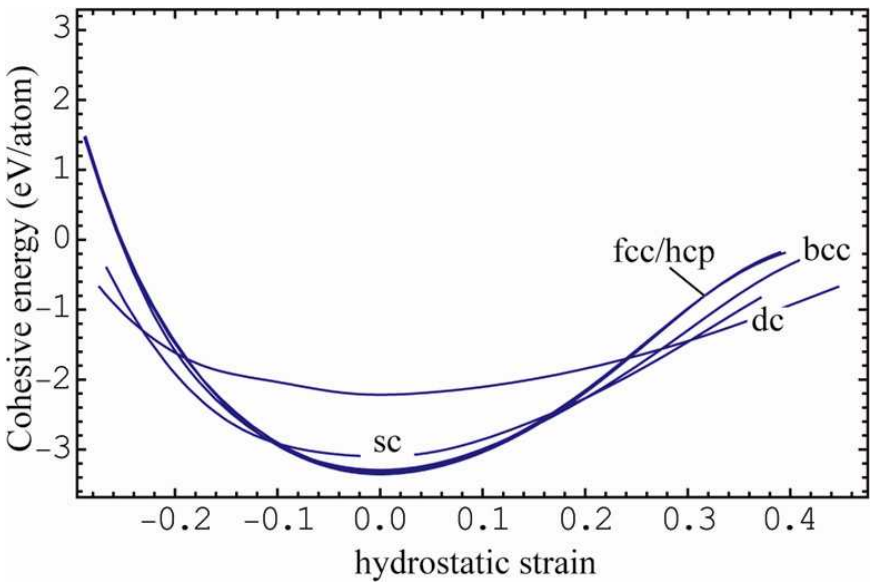
1. Properties (e.g., energies, geometries, and elastic constants) of a variety of clusters, lattices, surfaces, and defects are used to fit the parameters;
2. Four different optimization methods (conjugate gradients, differential evolution, simulated annealing, Nelder Mead simplex algorithm) are used in each fit to maximize probability of global minimum;
3. Parameters are constrained within first-principle motivated bounds;
4. Hundreds iterations with growth simulations as one of the drivers to guide the fitting.

Al Analytical Bond Order Potential

Matches DFT

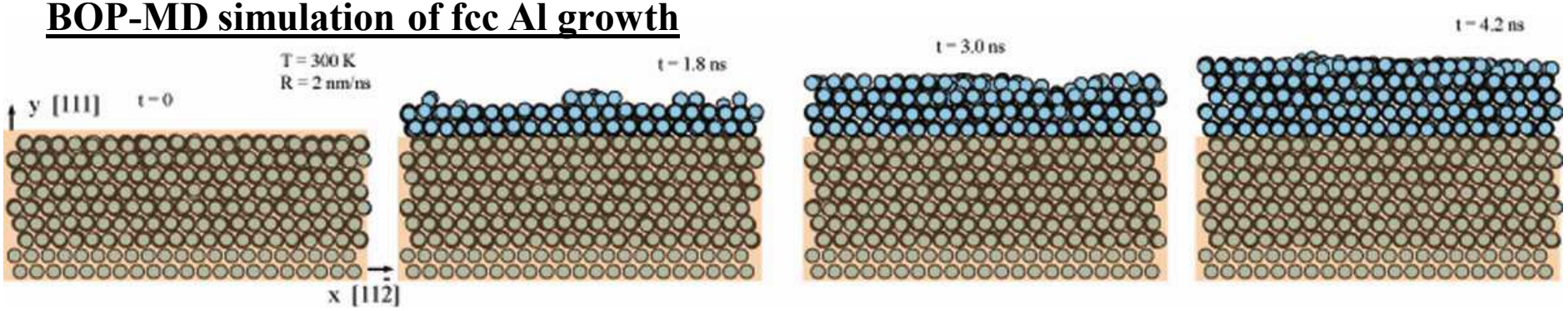


Smooth energy curves



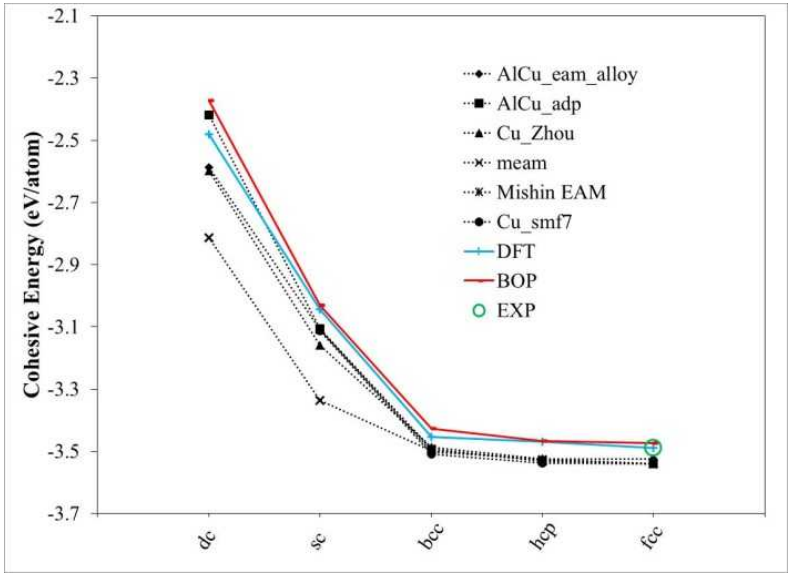
	EAM1	EAM2	ADP	MEAM	REAXFF1	REAXFF2	BOP	Exp.
$\gamma_{sf}(mJ/m^2)$	5	87	141	142	<1	<1	133	120-144

BOP-MD simulation of fcc Al growth

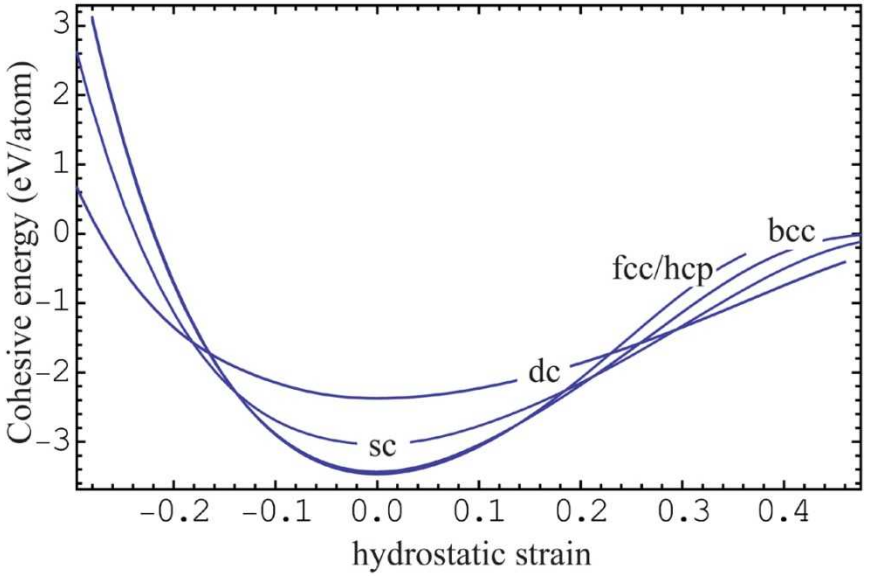


Cu Analytical Bond Order Potential

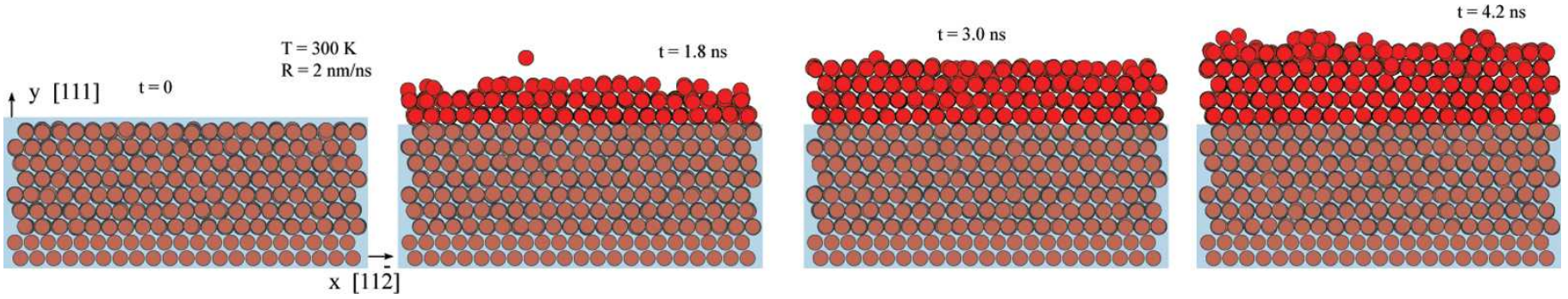
Matches DFT



Smooth energy curves

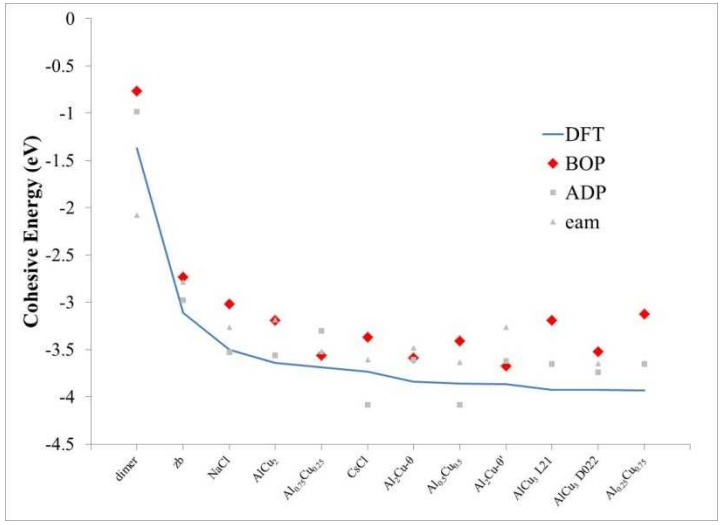


BOP-MD simulation of fcc Cu growth



Al-Cu Analytical Bond Order Potential

Matches DFT



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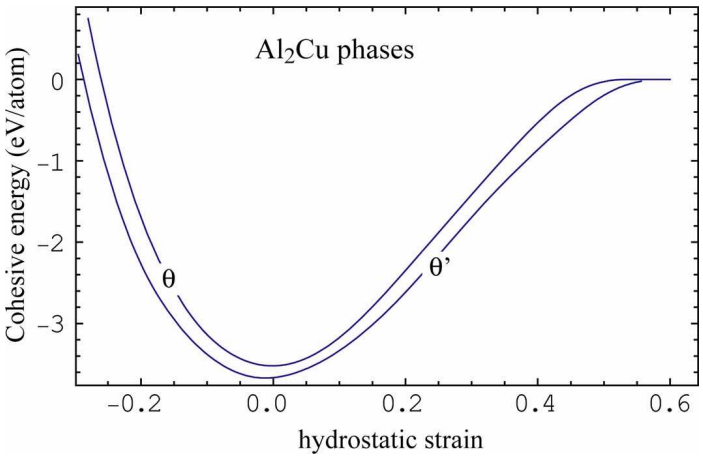
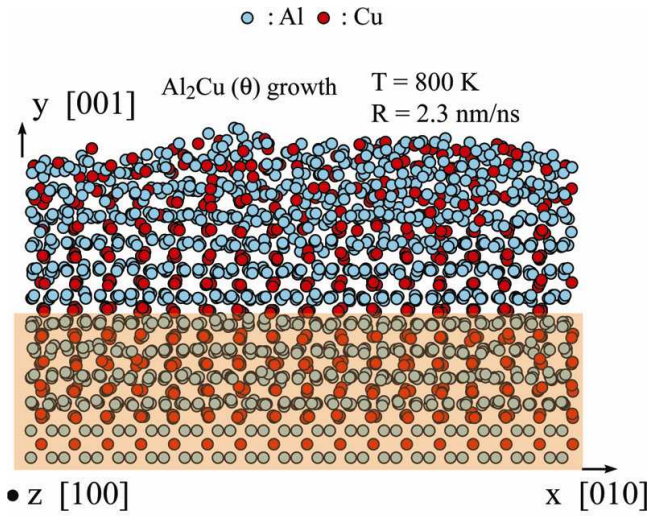
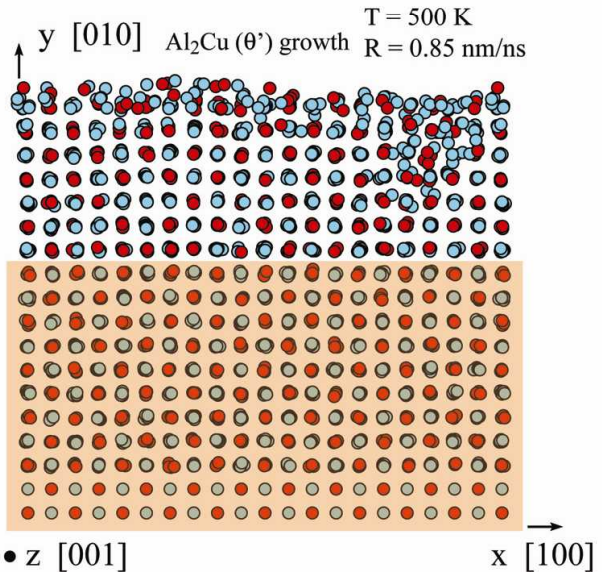


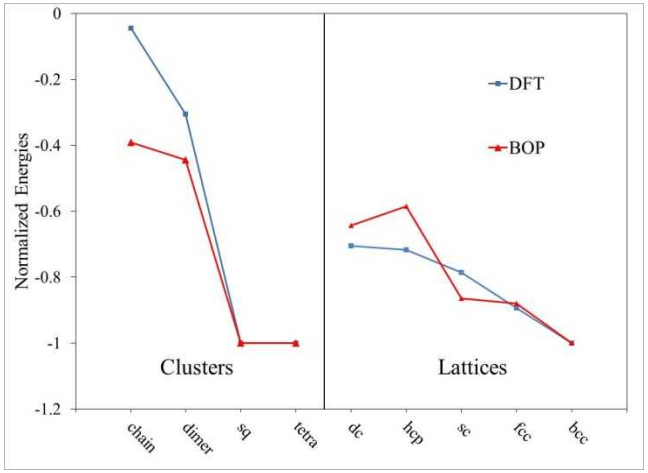
BOP-MD simulation of θ/θ' growth



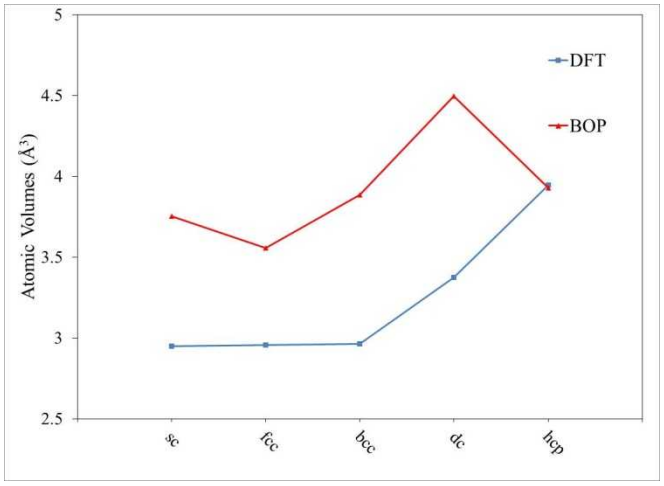


H Analytical Bond Order Potential

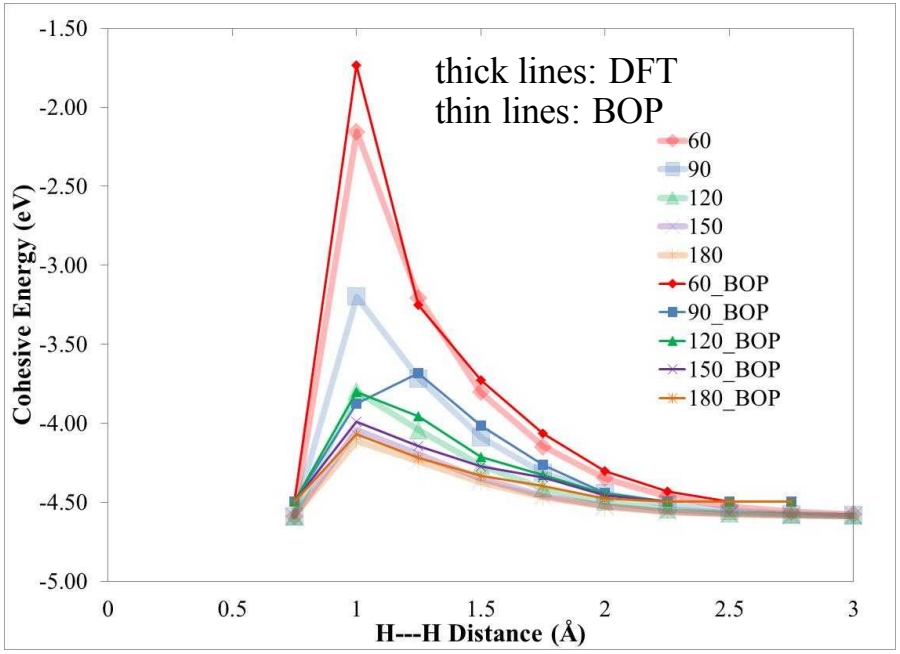
Cohesive energy trends of clusters and lattices

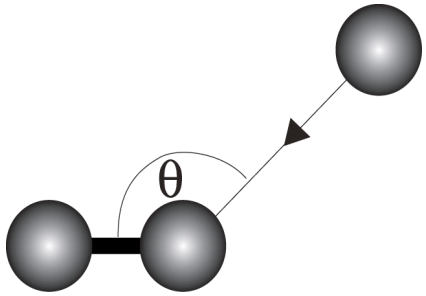


Atomic volume trends of lattices

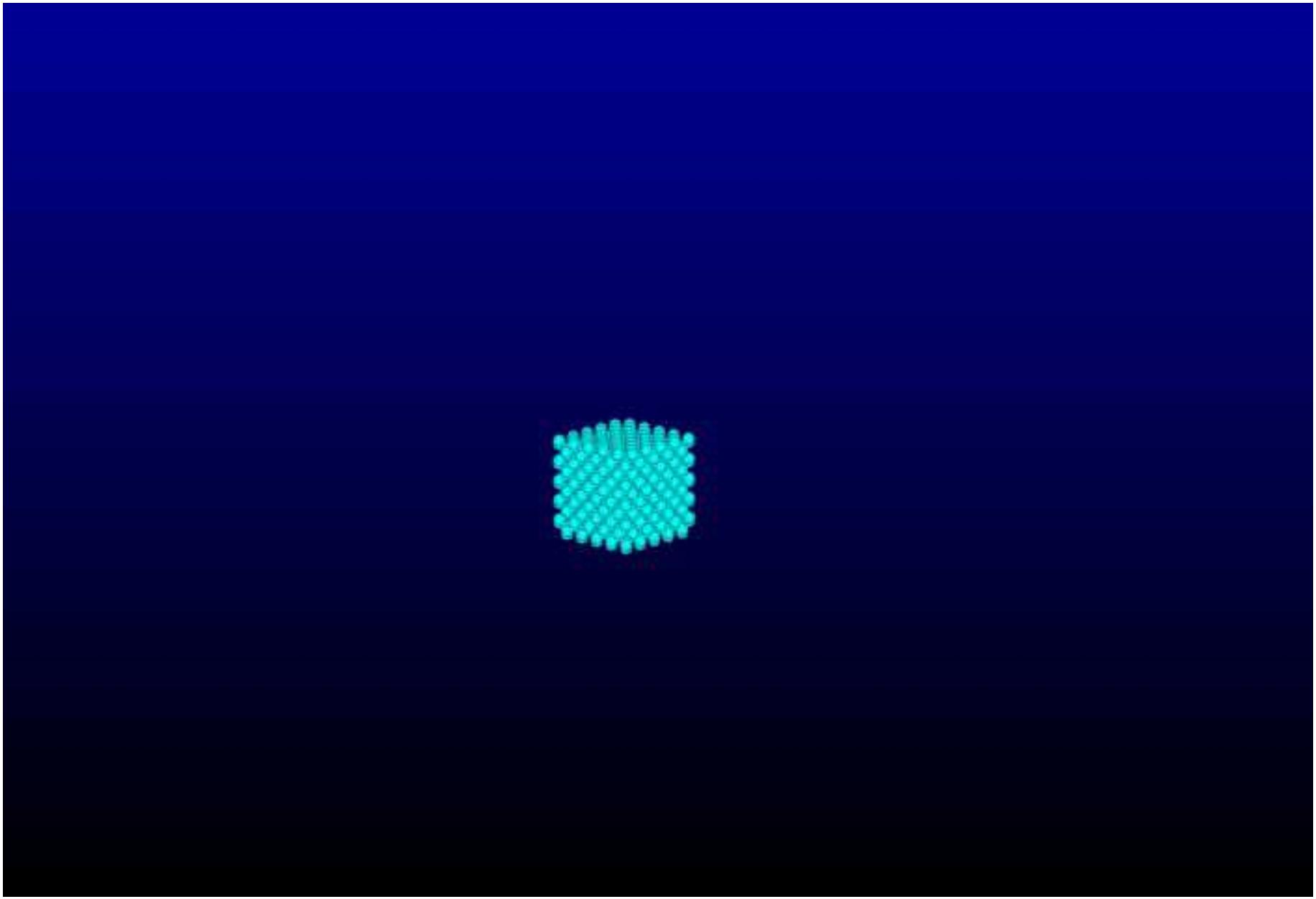


$H_2+H \rightarrow H+H_2$ energy profiles





H to H_2 Transformation Dynamics at 300 K



Published BOP Potentials

GaAs

1. D. A. Murdick, X. W. Zhou, H. N. G. Wadley, D. Nguyen-Manh, R. Drautz, and D. G. Pettifor, Phys. Rev. B, 73, 045206 (2006).
2. D. A. Murdick, H. N. G. Wadley, and X. W. Zhou, Phys. Rev. B, 125318 (2007).

CdZnTe

1. D K. Ward, X. W. Zhou, B. M. Wong, F. P. Doty, and J. A. Zimmerman, Phys. Rev. B, 85, 115206 (2012).
2. D. K. Ward, X. W. Zhou, B. M. Wong, F. P. Doty, and J. A. Zimmerman, Phys. Rev. B, 86, 245203 (2012).
3. X. W. Zhou, D. K. Ward, B. M. Wong, F. P. Doty, J. A. Zimmerman, G. N. Nielson, J. L. Cruz-Campa, V. P. Gupta, J. E. Granata, J. J. Chavez, and D. Zubia, Phys. Rev. B, 85, 245302 (2012).
4. J. J. Chavez, D. K. Ward, B. M. Wong, F. P. Doty, J. L. Cruz-Campa, G. N. Nielson, V. P. Gupta, D. Zubia, J. McClure, and X. W. Zhou, Phys. Rev. B, 85, 245316 (2012).
5. X.W. Zhou, D. K. Ward, B. M. Wong, and F. P. Doty, Phys. Rev. Lett., 108, 245503 (2012).

Available in LAMMPS

Conclusions

- Analytical BOPs have been developed for Al-Cu and separately for H;
- The Al-Cu BOP captures correctly the high stacking fault energy for Al, have smooth energy functions for elements and compounds, and predicts correctly the crystalline growth of both θ' and θ Al_2Cu compounds.
- The H BOP ensures the H_2 molecular gas as the equilibrium phase at the room temperature while predicts accurately the energy barriers for the $H + H_2 \rightarrow H_2 + H$ reactions with different H atom approaching directions;
- The Al-Cu-H-O BOP is currently under development.