NEW MEAM POTENTIALS FOR THE Al, Si, Mg, Cu, AND Fe ALLOY SYSTEM

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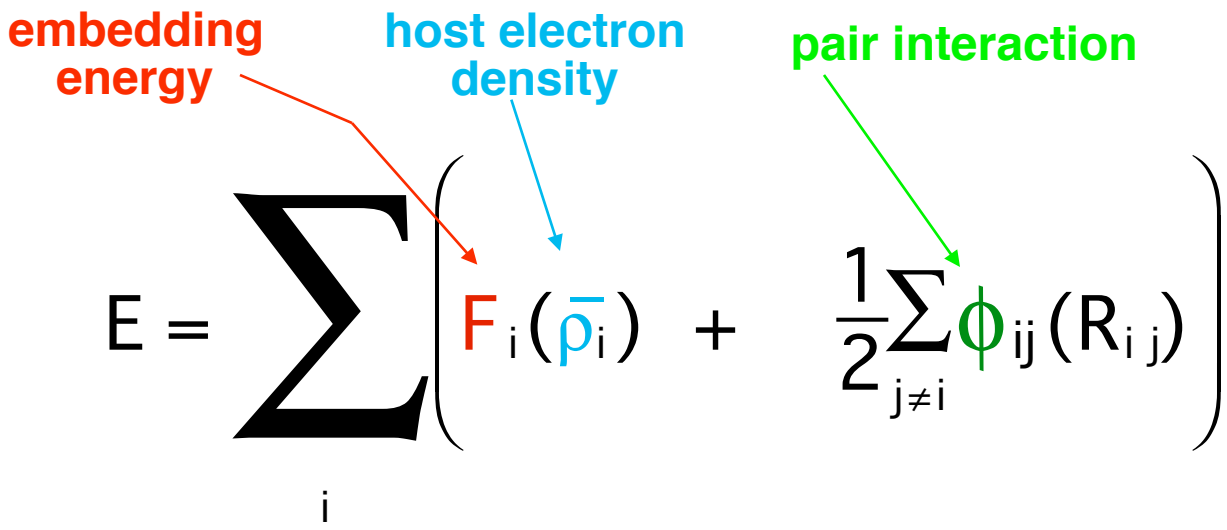
OUTLINE

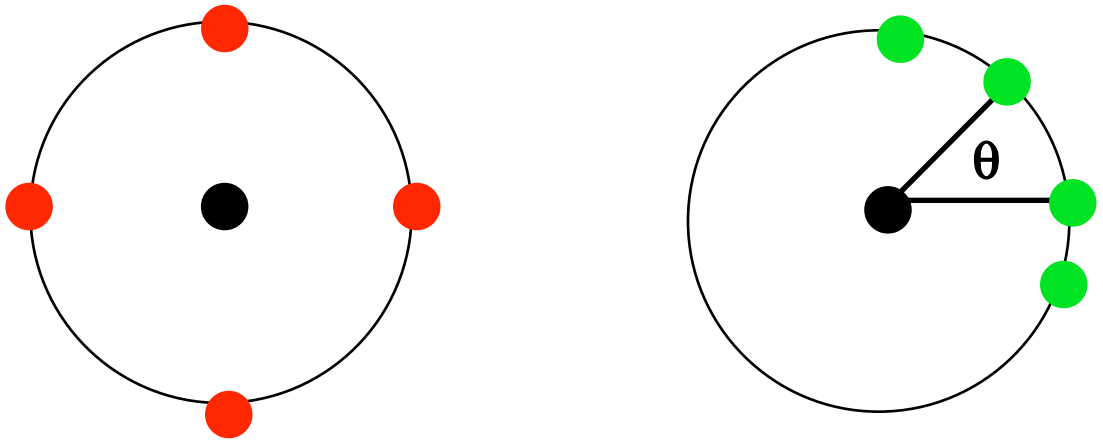
- Modified EAM (MEAM)
- Issues for multi-component systems
- Binary alloys calculations
- A few applications to the multi-component system

WE ARE ALL FAMILIAR WITH THE EMBEDDED ATOM METHOD FORMALISM



COMPLEX MATERIALS REQUIRE THE ADDITION OF ANGULAR FORCES

- **EAM uses a linear superposition of spherically averaged electron densities**
- **MEAM allows the background electron density to depend on the local symmetry**



MODIFIED EMBEDDED ATOM METHOD (MEAM)

Universal Binding Energy Relationship
UBER

$$E^u(R) = -E_c\left(1 + a^* + \delta a^{*3}\frac{r_e}{R}\right)e^{-a^*}$$

$$a^* = \alpha\left(\frac{R}{r_e} - 1\right) \qquad \alpha^2 = \frac{9\Omega B}{E_c}$$

Background Electron Density

$$\bar{\rho} = \rho^{(0)}\sqrt{1+\Gamma}$$

$$\Gamma = \sum_{l=1}^{3} t^{(l)}\left(\rho^{(l)}/\rho^{(0)}\right)^2$$

$$\rho_k^{(l)2} = \sum_i \rho_l(R_{ik}) \sum_j \rho_l(R_{kj}) P_l^0\left(\cos(\theta_{ikj})\right)$$

$$\rho_l = e^{-b^*} S \qquad b^* = \beta^{(l)}\left(\frac{\kappa}{r_e} - 1\right)$$

Embedding Function

$$F(\bar{\rho}) = AE_c\,\bar{\rho}\ln\bar{\rho}$$

Pair Potential

$$\phi(R) = \frac{2}{Z}\left\{E^u(R) - F(\bar{\rho}^0(R))\right\}S$$

12 parameters + angular screening for the pair potential and electron densities

A FOUR PARAMETER MEAM MODEL HAS BEEN DEVELOPED FOR BINARY ALLOYS

- **Use previously developed functions for elements A and B**
- **Electron density ratio (A/B)**
- **Universal EOS for reference structure, AB (B1)**

$$E = -E_0\left(1 + a^*\right)e^{-a^*} \qquad a^* = \alpha\left(r/r_0 - 1\right)$$

  - **-nearest neighbor distance, r_0 (Å)**
  - **-distance scaling, α**
  - **-formation energy, E_0 (eV/atom)**
- **Angular screening**

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ELECTRON DENSITY SCALING PARAMETER IS LOST FOR MULTI-COMPONENT SYSTEMS

- For A-B system: ρ^0_B / ρ^0_A
- For A-C system: ρ^0_C / ρ^0_A
- For B-C system: ρ^0_C / ρ^0_B

- For A-B-C system: ρ^0_B / ρ^0_A, ρ^0_C / ρ^0_A
- For an N-component system
  - ✓ N(N-1)/2 binaries
  - ✓ 3N(N-1)/2 + (N-1) alloy parameters
- Angular screening
  - ✓ 8N(N-1)/2 alloy parameters

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SINGLE ELEMENT PARAMETERS

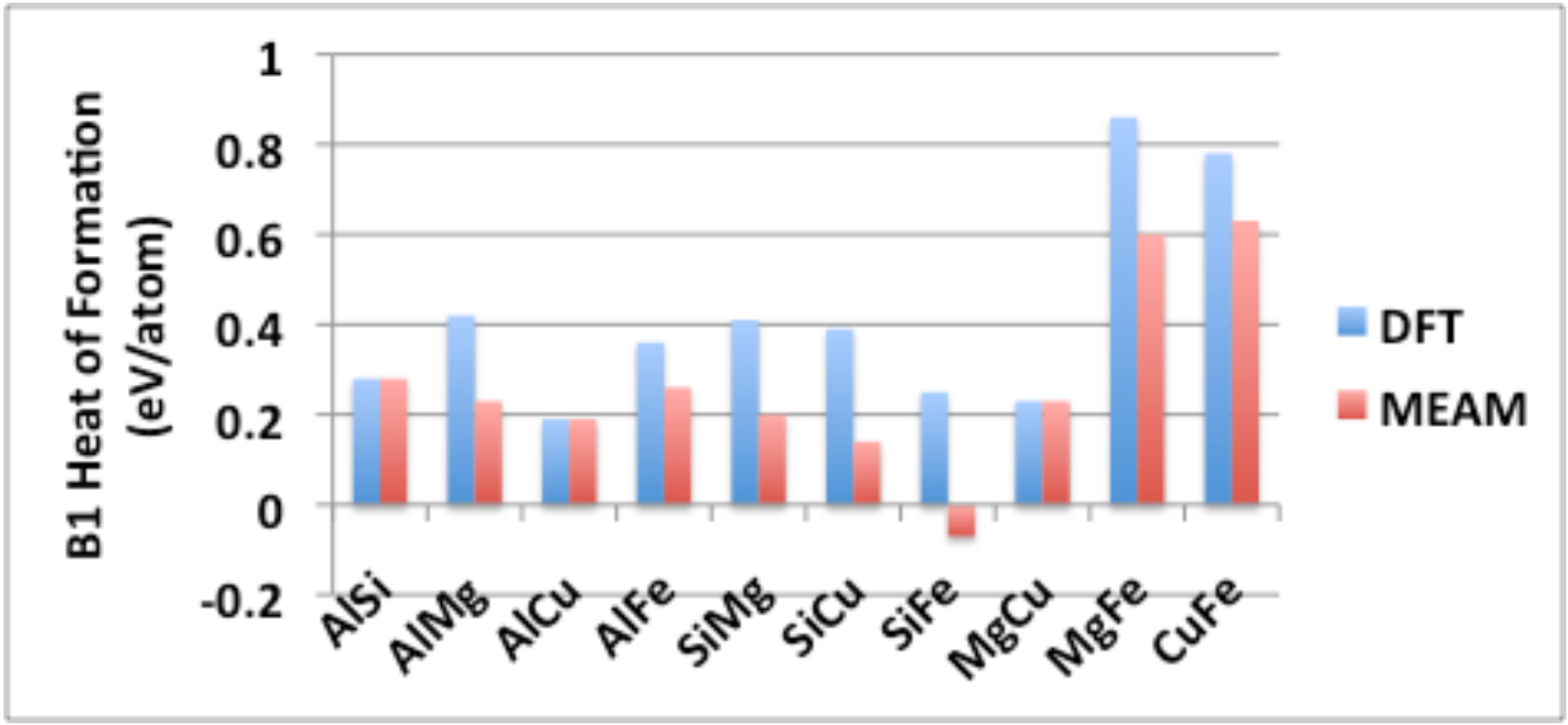
elem.	E_c[eV]	a_0[Å]	A	α	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	$\beta^{(3)}$	$t^{(0)}$	$t^{(1)}$	$t^{(2)}$	$t^{(3)}$	$C_{\min}$	$C_{\max}$	ρ_0
Al	3.353	4.05	1.07	4.64	2.04	1.5	6.0	1.5	1.0	4.00	-2.30	8.01	0.8	2.8	1.0
Si	4.63	5.431	1.00	4.87	4.4	5.5	5.5	5.5	1.0	2.05	4.47	-1.80	2.0	2.8	2.2
Mg	1.51	3.194	0.8	5.52	4.0	3.0	0.2	1.2	1.0	10.04	9.49	-4.3	0.8	2.8	0.63
Cu	3.54	3.62	1.07	5.11	3.634	2.2	6.0	2.2	1.0	4.91	2.49	2.95	0.8	2.8	1.1
Fe	4.28	2.851	0.555	5.027	3.5	2.0	1.0	1.0	1.0	-1.6	12.5	-1.4	0.8	1.9	1.0

For Fe the δ parameter in the EOS was used

ALLOY PARAMETERS

X	Y	ΔH_{B1}^{XY} [eV]	r_e[Å]	α	C_{min}^{XYX}	C_{max}^{XYX}	C_{min}^{YXY}	C_{max}^{YXY}	C_{min}^{XXY}	C_{max}^{XXY}	C_{min}^{XYY}	C_{max}^{XYY}
Al	Si	0.28	2.62	4.56	0.5	2.8	2.0	2.8	2.0	2.8	2.0	2.8
Al	Mg	0.23	2.87	4.52	2.0	2.8	0.0	2.8	2.0	2.8	0.0	2.8
Al	Cu	0.19	2.53	4.65	0.0	2.8	2.0	2.8	2.0	2.8	2.0	2.8
Al	Fe	0.26	2.45	4.64	0.9	2.8	0.1	2.8	2.0	2.8	2.0	2.8
Si	Mg	0.20	2.75	4.73	1.0	2.8	1.0	2.8	2.0	2.8	2.0	2.8
Si	Cu	0.14	2.46	4.74	0.0	2.8	0.0	2.8	2.0	2.8	2.0	2.8
Si	Fe	-0.07	2.39	5.17	1.0	2.8	1.0	2.8	2.0	2.8	0.0	2.8
Mg	Cu	0.23	2.63	4.70	2.0	2.8	0.0	2.8	2.0	2.8	2.0	2.8
Mg	Fe	0.60	2.61	4.96	0.65	2.8	0.0	2.8	2.0	2.8	2.0	2.8
Cu	Fe	0.63	2.42	5.21	2.0	2.8	0.0	2.8	2.0	2.8	2.0	2.8

MEAM COMPARISON TO DFT DATA BASE



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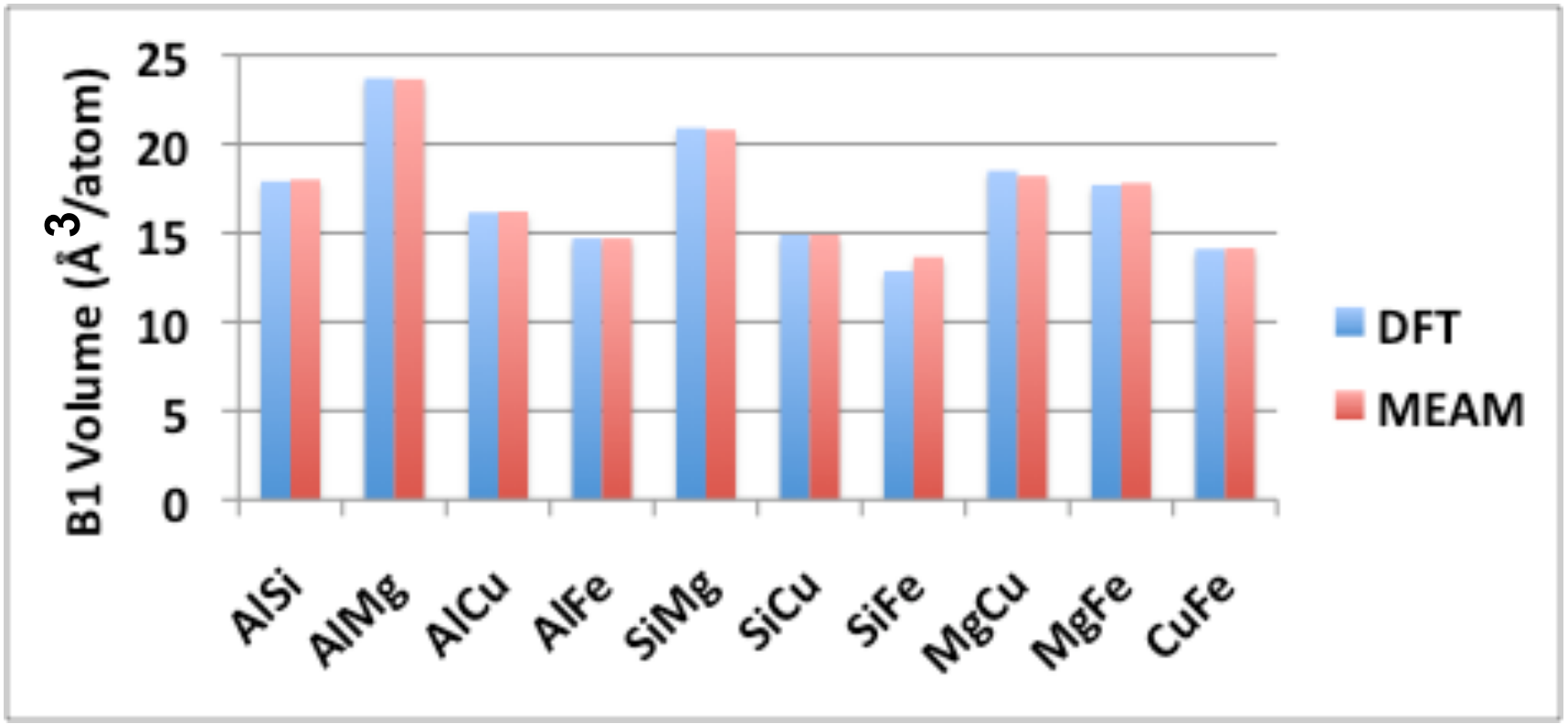

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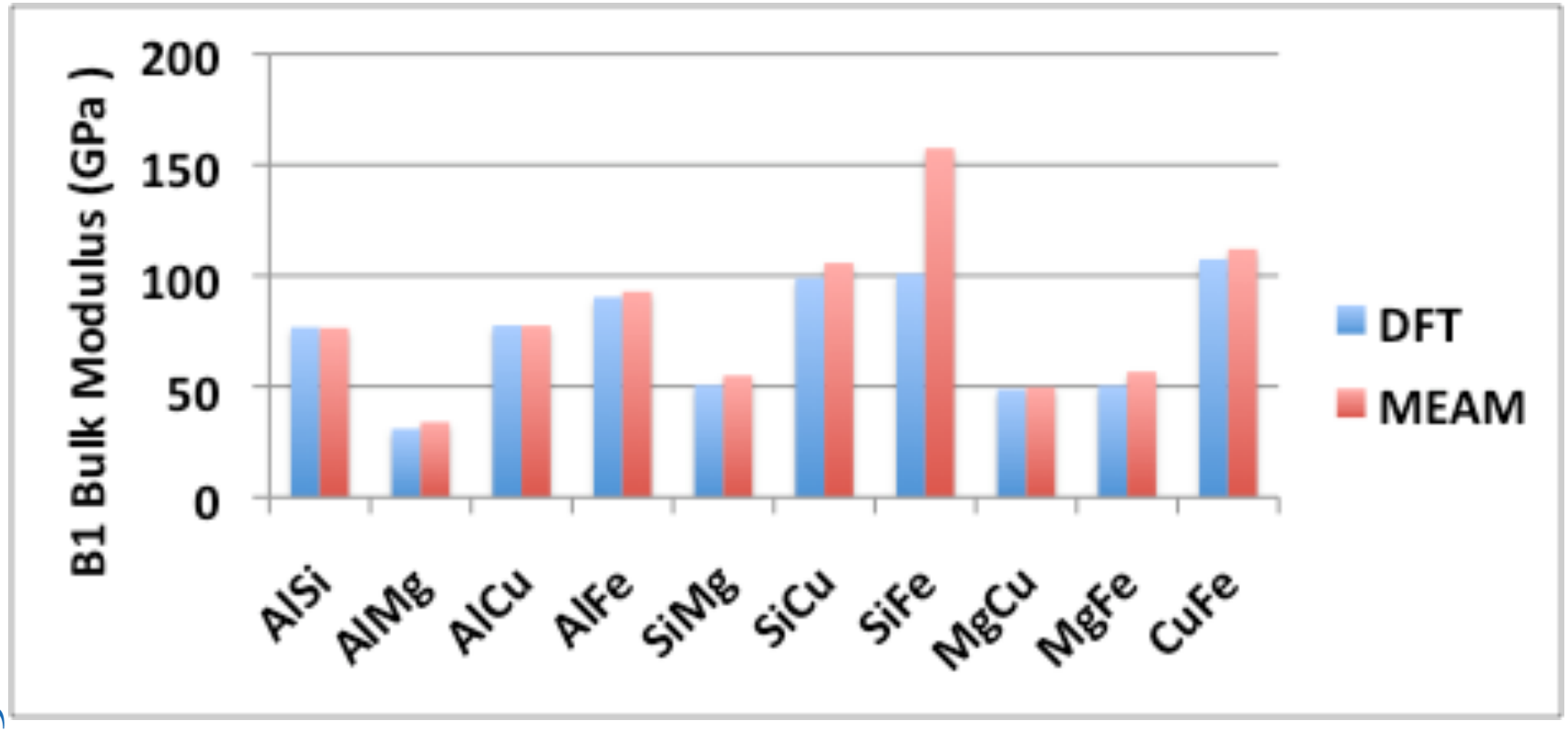

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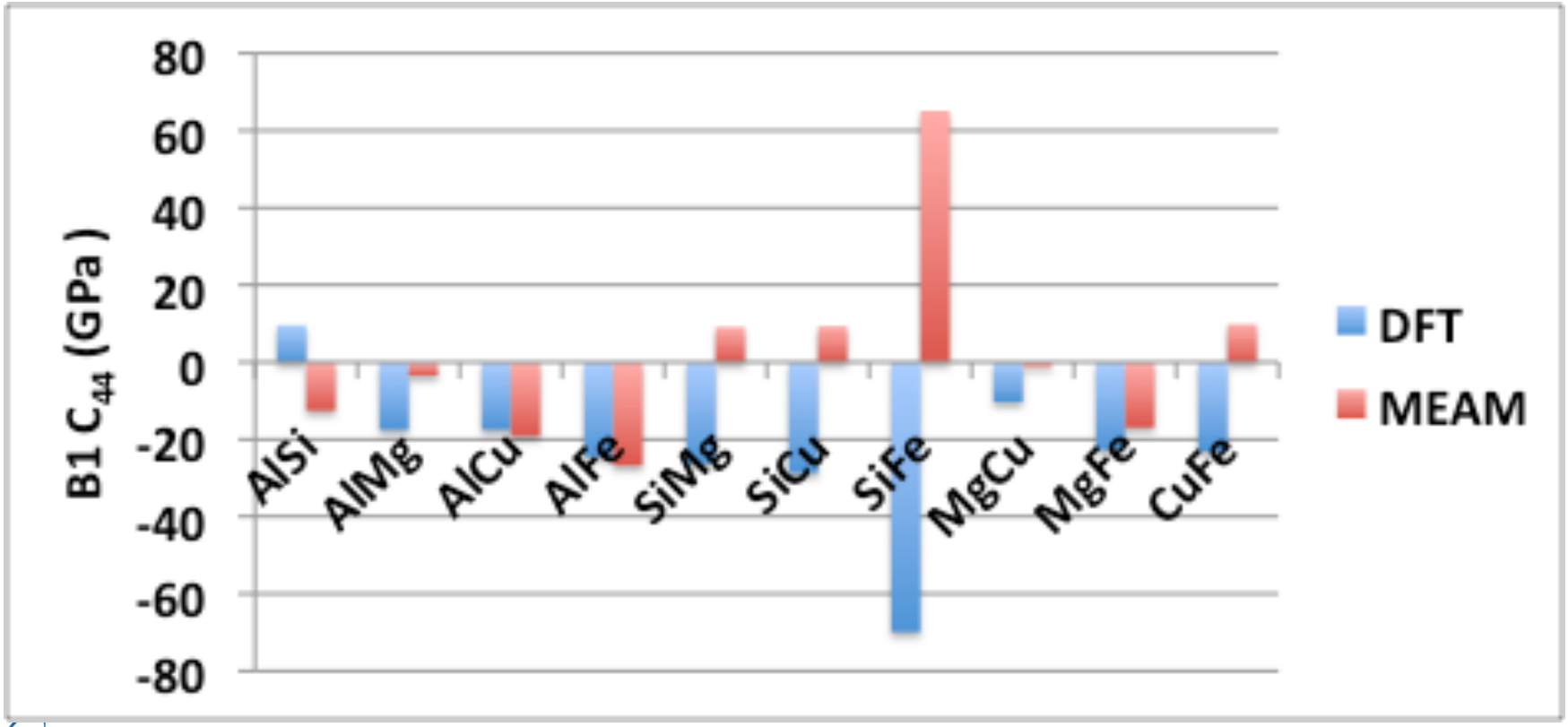

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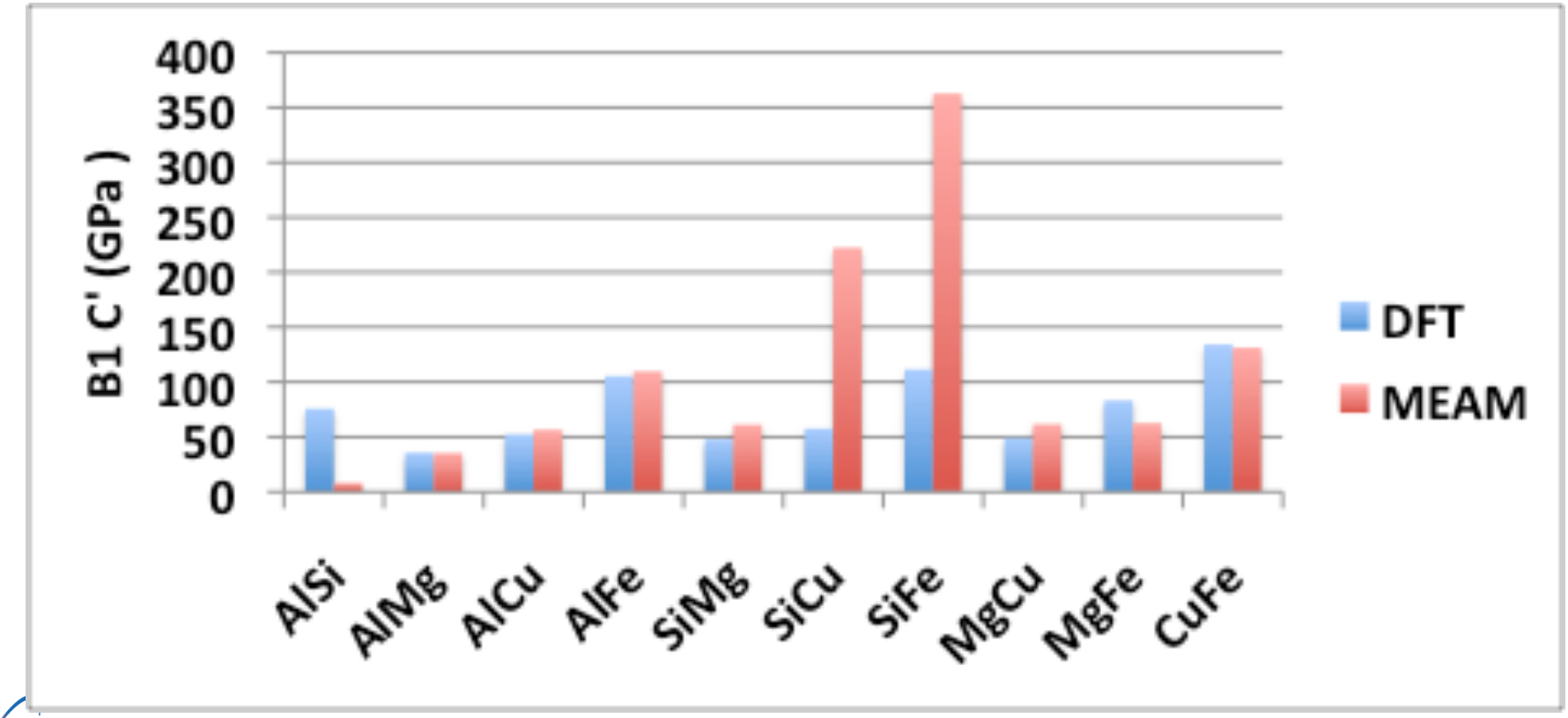
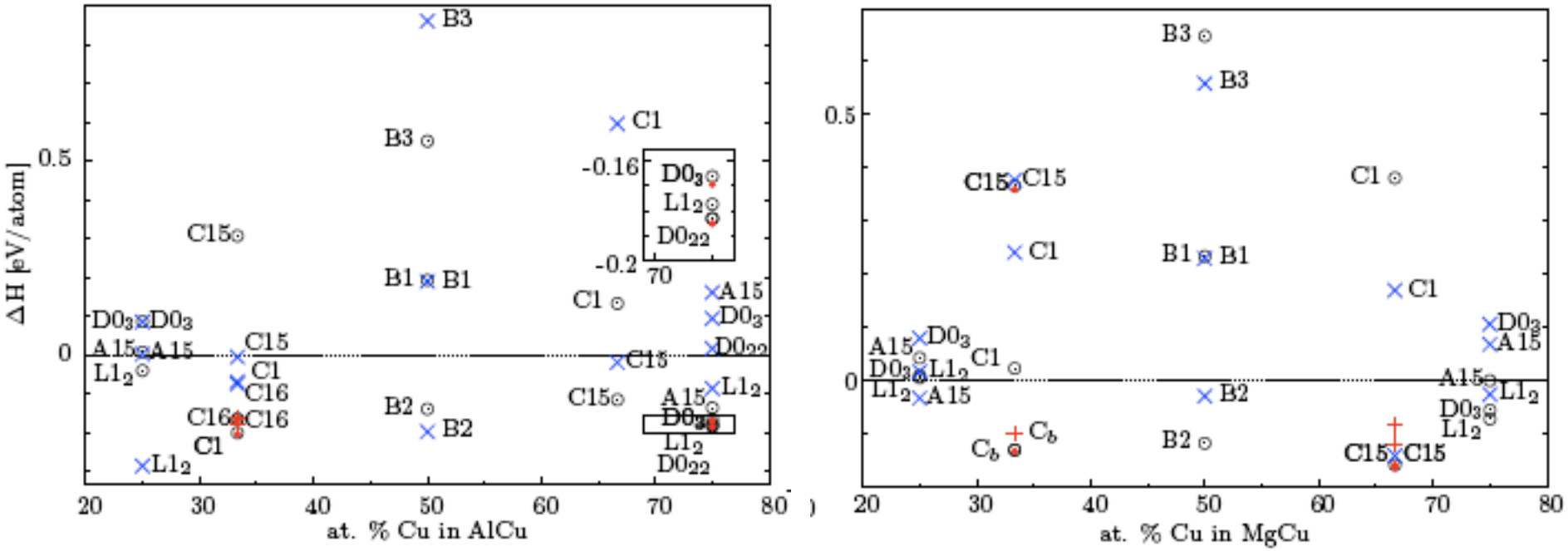


CALCULATED HEATS AGREE WITH EXPERIMENT AND DFT OVER THE ENTIRE COMPOSITION RANGE



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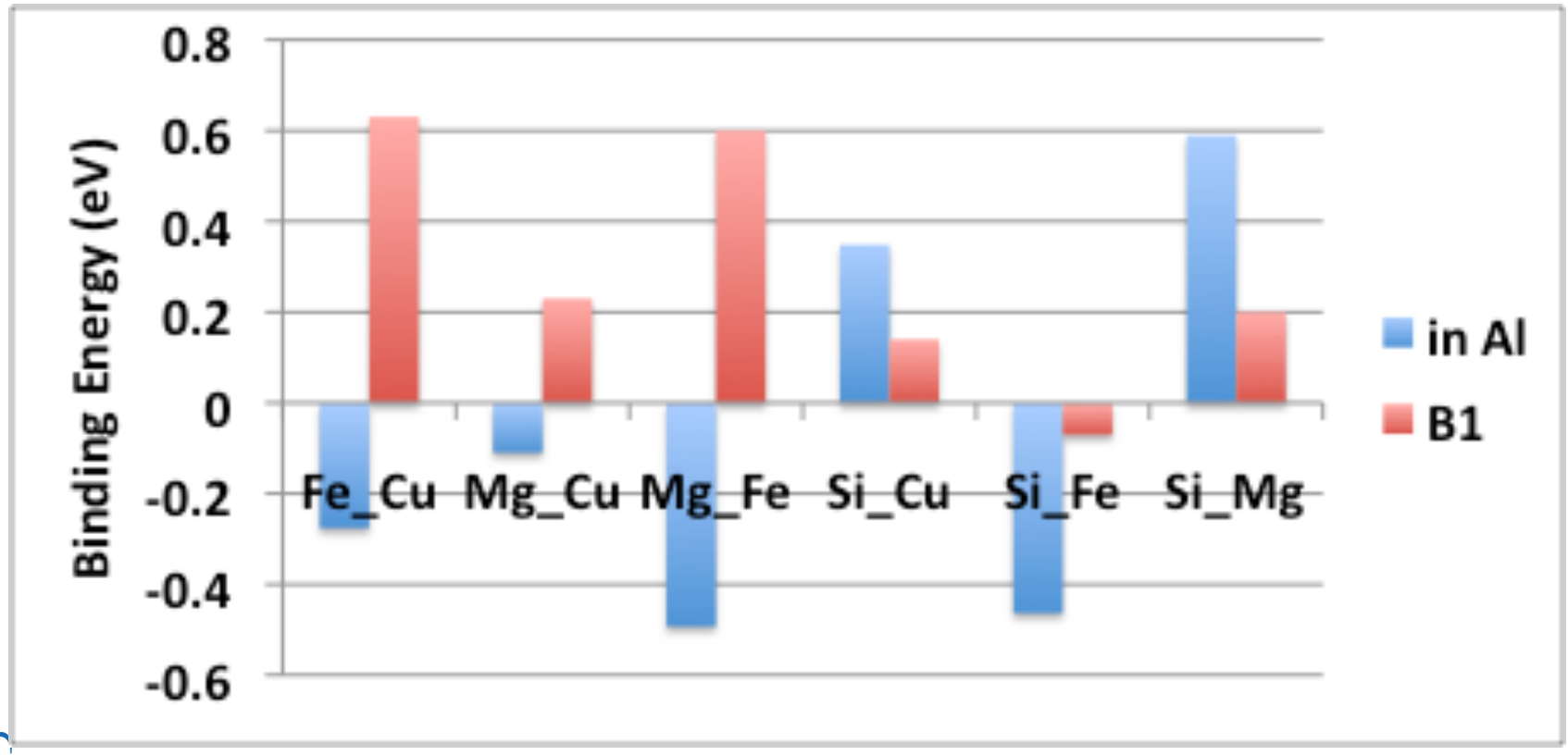
PREDICTED SOLUTION ENERGY AGREES REASONABLY WELL WITH DFT

Bulk	Substitute atom				
	Al	Si	Mg	Cu	Fe
Al		0.5 (0.5)	0.06 (0.05)	−1.1 (−0.1)	−1.2(−0.4)
Si	6.6 (0.9)		2.9 (2.4)	1.9 (2.)	1.6 (1.9)
Mg	−0.7 (0.06)	0.2 (0.4)		−0.2 (0.2)	1.5 (1.1)
Cu	0.8 (−0.7)	0.8 (−0.2)	1.1 (−0.2)		2.9 (1.4)
Fe	0.8 (−0.7)	−2.9 (−1.1)	0.8 (1.0)	−0.3 (0.8)	

BINDING OF SUBSTITUTIONAL IMPURITIES NOT REFLECTED BY B1 STABILITY



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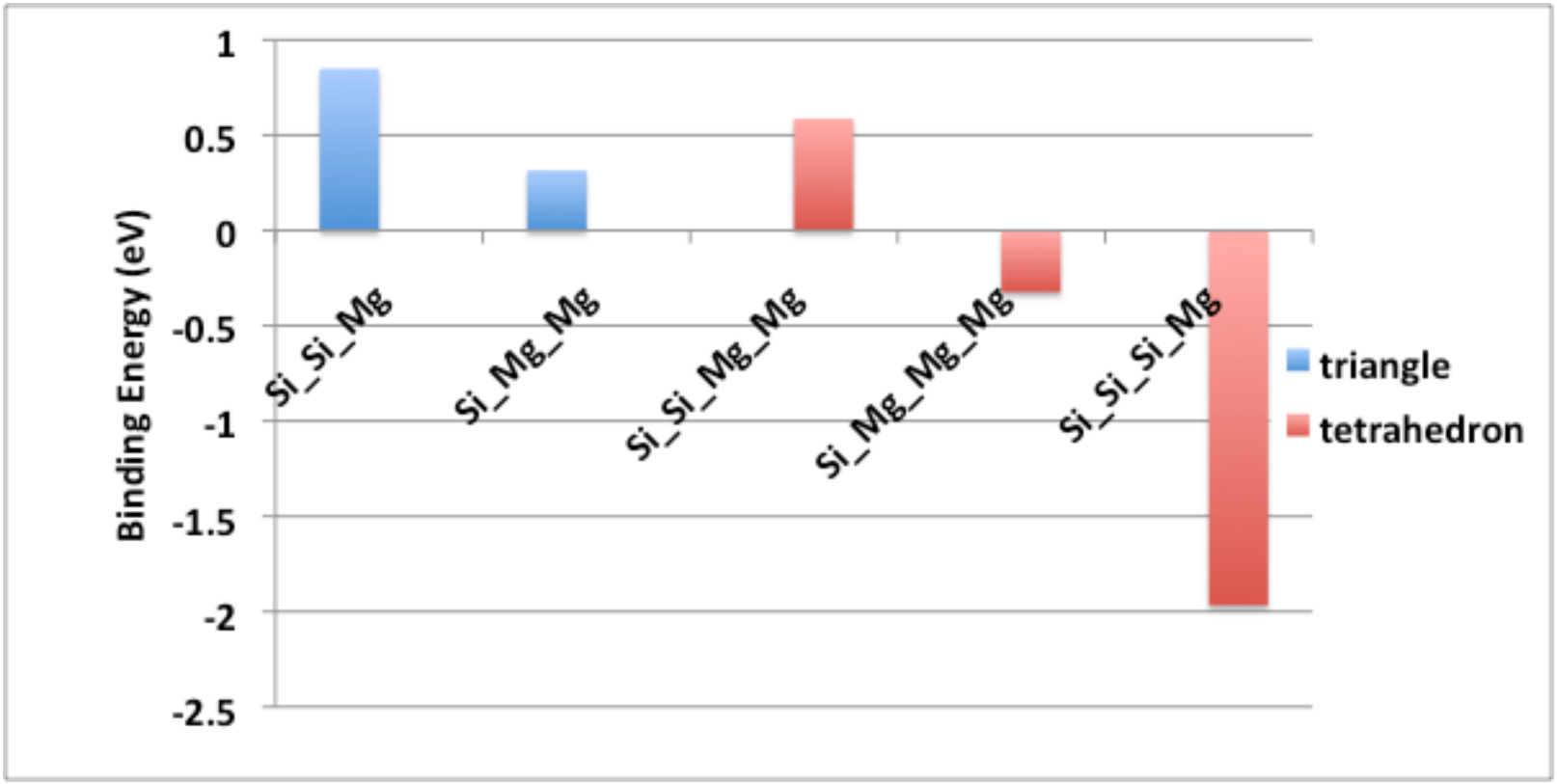
SMALL CLUSTERS OF Si AND Mg in Al ARE BOUND



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SUMMARY

- **MEAM potentials were developed for a 5 component system: Al, Si, Mg, Cu, and Fe**
- **Calculations show the functions reproduce the DFT and experimental data base**
- **Small clusters of Si and Mg are shown to be stable in Al**