Development and Application of Charge Optimized Many-Body (COMB) Potentials for Surface Chemistry and Heterogeneous Material Interfacial Interactions

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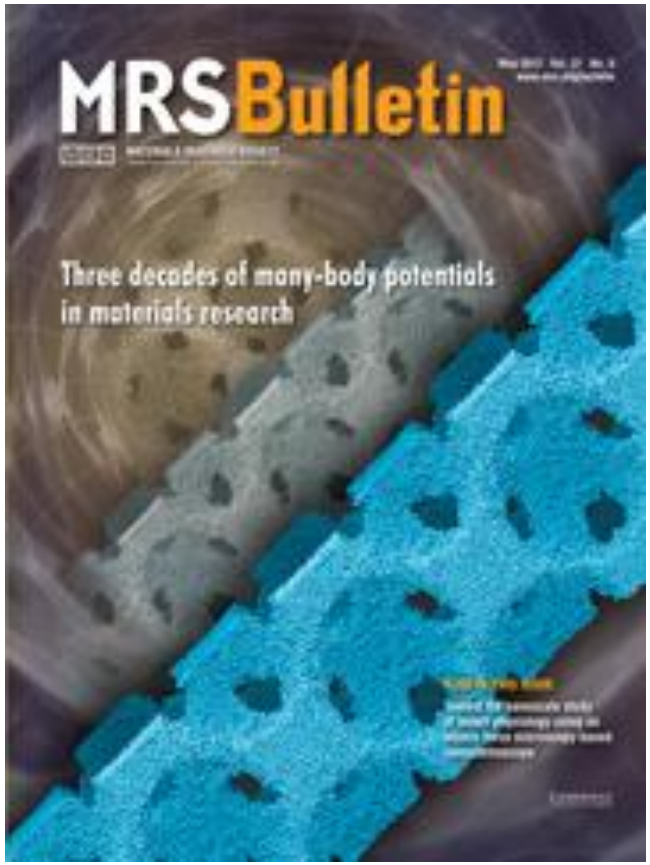
Reactive many-body empirical potentials in materials science



May 2012 issue

Historically developed for materials with specific types of chemical bonds

- Tersoff potentials for Si
  - Brenner or REBO potential for C,H + O,F,S,….
  - AIREBO
- EAM potentials for metals
  - MEAM for metals and oxides
  - EAM+ES for metals and oxides
- Buckingham potentials for ionically bound materials

Classical Potential Forms

$$V_{LJ} = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$= \varepsilon \left[\left(\frac{r_m}{r}\right)^{12} - 2\left(\frac{r_m}{r}\right)^{6}\right]$$

Lennard-Jones potential

$$V_{ij}(r_{ij}) = V_{repulsive}(r_{ij}) + b_{ijk} V_{attractive}(r_{ij})$$

Bond-order potential (Tersoff, Brenner, REBO, etc.)

$$E_i = F_\alpha\left(\sum_{i \neq j} \rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{i \neq j} \phi_{\alpha\beta}(r_{ij})$$

Embedded Atom Method (EAM) potential

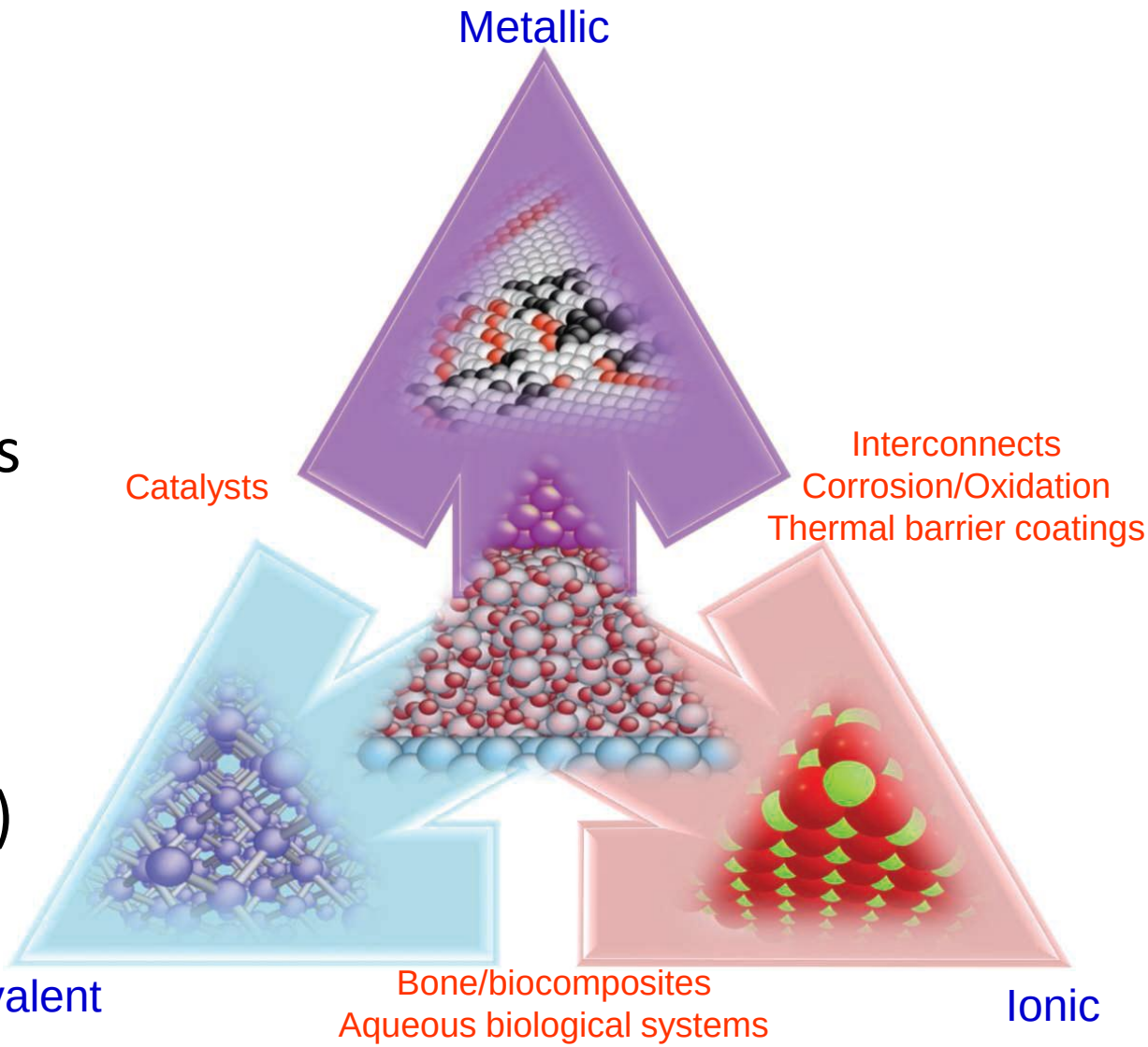
$$V_{ij}(r) = A_{ij} \exp\left(-\frac{r}{\rho_{ij}}\right) - \frac{C_{ij}}{r^6}$$

Buckingham potential

Equations from Wikipedia, October, 2012

Modeling Multicomponent Systems

- Inherent to many applications
- Challenge for traditional reactive empirical potentials (force fields)
- Developed the charge optimized many body (COMB) potential to model heterogeneous systems



S. R. Phillpot, S. B. Sinnott, ***Science*** 325, 1634 (2009).

Development

Overview of COMB Implementations

- 1st generation[1] (COMB1)
  - Si/SiO_2, Cu, Al
- 2nd generation[2](COMB2) In LAMMPS, available
  - Si/SiO_2, $Cu/Cu_2O/CuO$, Hf/HfO_2, Ti/TiO_2
- 3rd generation[3](COMB3) In LAMMPS, will be released shortly
  - C/H/O/N, $Cu/Cu_2O/CuO$, Zr/ZrO_2, Zn/ZnO, U/UO_2, $Al/Al_2O_3/AlN$, $Ti/TiN/TiO_2$, Pt, $PbTiO_3$

[1] J. **Yu**, et. al., *Phys. Rev. B* 75 085311 (2007)
[2] T.-R. **Shan**, et al., *Phys. Rev. B* **81**, 125328 (2010).
[3] T. **Liang**, et al., *Journal of Physical Chemistry A* **116**, 7976 (2012).

Functional Form of COMB Potential

General formalism:

$$E_T = \sum_i \left[E_i^S(q_i) + \frac{1}{2}\sum_{j\neq i} V_{ij}\left(r_{ij}, q_i, q_j\right) + B_i(q_i) + C_i(r_{ij}, \theta_{jik}) \right]$$

- Self energy: fit to atomic ionization energies and electron affinities
  - $E_i^S(q_i) = \chi_i q_i + J_i q_i^2 + K_i q_i^3 + L_i q_i^4$
  - Penalty function to capture change in self energy due to field of ionic lattice
    - $E_i^{field}(r, q_j) = \sum_{j\neq i}^{NN} \left(\frac{\rho_1 q_j}{r_{ij}^5} + \frac{\rho_2 q_j^2}{r_{ij}^5} \right)$

J. **Yu**, S. B. **Sinnott**, S. R. **Phillpot**, *Phys. Rev. B* 75 085311 (2007)
T.-R. **Shan**, B. D. **Devine**, T. W. **Kemper**, S. B. **Sinnott**, S. R. **Phillpot**, *Phys. Rev. B* 81 125328 (2010)

Functional Form of COMB Potential

- $V_{ij}(r_{ij},q_i,q_j) = f_c(r_{ij})\cdot A_{ij}(q_i,q_j)\cdot e^{-\lambda_{ij}\cdot r_{ij}} - f_c(r_{ij})\cdot b_{ij}\cdot B_{ij}(q_i,q_j)\cdot e^{-\alpha_{ij}\cdot r_{ij}} + q_i\cdot J_{ij}(r_{ij})\cdot q_j$
- Short range interactions: Tersoff type made charge dependent
  - A change in the partial charge on an atom affects the effective ionic radius, which influences the short-range repulsion and attraction
  - $A_{ij}(q_i,q_j) = A_{ij}\cdot\exp\left[\lambda_i D_i(q_i)+\lambda_j D_j(q_j)\right]$ → repulsive
  - $B_{ij}(q_i,q_j) = B_{ij}\cdot B^*_{ij}(q_i,q_j)\cdot\exp\left[\alpha_i D_i(q_i)+\alpha_j D_j(q_j)\right]$ → attractive
- Bond order term, b_{ij}, includes many-body effect
  - $b_{ij} = \left[1+\left(\beta_i\sum_{k\neq i,j}\xi_{ijk}\,g(\theta_{jik})\right)^{n_i}\right]^{-1/(2n_i)}$
  - $\zeta_{ijk} = f_{S_{ik}}\,e^{\left[\alpha_{ij}^{m_i}\left(r_{ij}-r_{ik}\right)^{m_i}\right]}$ → symmetry function
  - $g(\theta_{jik}) = 1+c_i^2/d_i^2 - c_i^2/\left[d_i^2+\left(h_i-\cos\theta_{jik}\right)^2\right]$ → angular function

J. **Yu**, S. B. **Sinnott**, S. R. **Phillpot**, *Phys. Rev. B* 75 085311 (2007)
T.-R. **Shan**, B. D. **Devine**, T. W. **Kemper**, S. B. **Sinnott**, S. R. **Phillpot**, *Phys. Rev. B* 81 125328 (2010)

Functional Form of COMB Potential

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- Long range interactions: Coulomb electrostatics
  - Spherical charge distribution: 1*s*-type Slater orbital
  - $J_{ij}(r_{ij}) = n_{ij}\int d^3r_i \int d^3r_j\ \rho_i(r_i,q_i)\rho_j(r_j,q_j)/r_{ij}$
  - $\rho_i(r_i,q_i) = q_i\dfrac{\xi_i^3}{\pi}\exp\left(-2\xi_i\left|r-r_i\right|\right)$
  - Treats long range interactions with Wolf summation

D. **Wolf**, P. **Keblinski**, S. R. **Phillpot**, and J. **Eggebrecht**, J. Chem. Phys. 110, 8254 (1999)
J. **Yu**, S. B. **Sinnott**, S. R. **Phillpot**, *Phys. Rev. B* 75 085311 (2007)
T.-R. **Shan**, B. D. **Devine**, T. W. **Kemper**, S. B. **Sinnott**, S. R. **Phillpot**, *Phys. Rev. B* 81 125328 (2010)

Most Recent Modifications

- Extended to include:
  - Organic molecules: C/H/O/N, NO_x
  - Oxides and nitrides: ZrO_2, ZnO, UO_2, TiN, AlN, Al_2O_3

- $$E_T = \sum_i \left[E_i^S(q_i) + \frac{1}{2}\sum_{j\neq i} V_{ij}\left(r_{ij}, q_i, q_j\right) + B_i(q_i) + C_i(r_{ij}, \theta_{jik}) + E^{polar}(q_i, ri_j) + E^{vdW}(r_{ij}) \right]$$

  - $$E^{Polar}[q_i, r_{ij}] = \sum_i \frac{\vec{\mu}_i^2}{2\alpha_i} + \sum_i \vec{\mu}_i \cdot \vec{E}_i^q + \tfrac{1}{2}\sum_i \sum_{j\neq i} \vec{\mu}_i T_{ij} \vec{\mu}_j$$ → *polarization*

  - $$b_{ij} = \left[1 + \left(\sum_{j\neq i}^{N} \sum_{k\neq i,j}^{N} \zeta_{ijk}\, g(\cos(\theta_{ijk})) + P_{ij}\left(N_i^1, N_i^2, N_i^3 \ldots\right) \right)^{\eta_i} \right]^{\frac{-1}{2\eta_i}} + b_{ij}^{\pi} + b_{ij}^{DH}$$

modified angular

tri-cubic spline coordination

radicals and dihedrals

Bond Order for COMB C/H/O - Radicals and Aromatics

$$b_{ij}^{\pi} = \pi_{ij}(\Omega_i, \Omega_j, N_{ij}^{conjug})$$

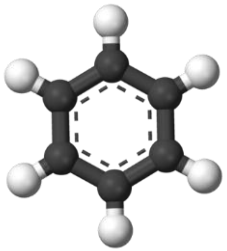
π_{ij} is a tri-cubic spline function

T_{ij} is the induced dipole field tensor

$$N_{ij}^{conjug} = 1 + \left[\sum_{k \neq ij}^{carbon} F_C(r_{ik}) T_{ik} P(X_{ik})\right]^2 + \left[\sum_{l \neq ij}^{carbon} F_C(r_{jl}) T_{jl} P(X_{jl})\right]^2$$

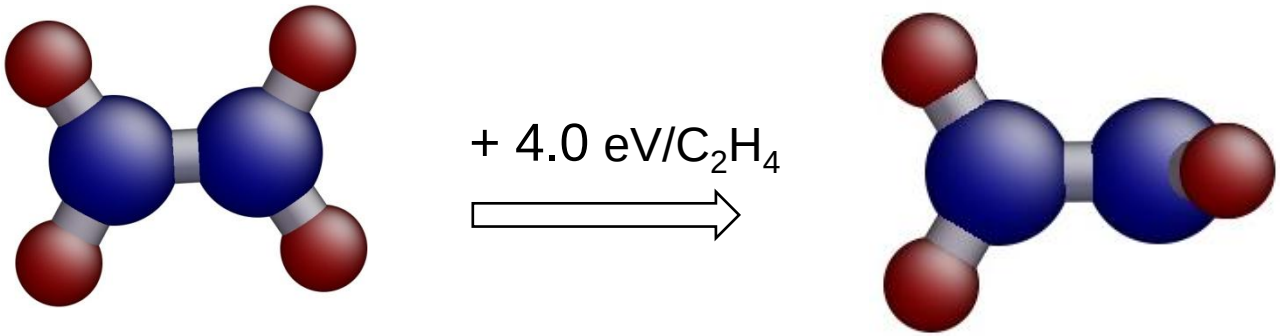
$$P(X_{ik}) = \begin{cases} 1 & X_{ik} < 2 \\ \frac{1}{2}\left[1 + \cos\left(\pi(X_{ik} - 2)\right)\right] & 2 < X_{ik} < 3 \\ 0 & X_{ik} > 3 \end{cases} \quad \text{and} \quad X_{ik} = \Omega_k$$

Ω_i is the coordination number of i^{th} atom



$$\Longrightarrow \quad \pi_{ij}(2,2,3)$$

Bond Order for COMB C/H/O - Torsion Term



Θ_{ijkl} : dihedral angle

$$b_{ij}^{DH} = \phi_{ij}(\Omega_i, \Omega_j, N_{ij}^{conjug}) \left[\sum_{k \neq i,j} \sum_{l \neq i,j} (1 - \cos^2(\Theta_{ijkl})) F_C(r_{ik}) F_C(r_{jl}) \right]$$

$\phi_{ij}(\Omega_i, \Omega_j, N_{ij}^{conjug})$

ϕ_{ij} is a tri-cubic spline function

Cost of Potentials in LAMMPS

Potential	System	# Atoms	Memory	LJ Ratio
Lennard-Jones	LJ liquid	32000	12 Mb	1.0x
EAM	bulk Cu	32000	13 Mb	2.4x
Tersoff	bulk Si	32000	9.2 Mb	4.1x
Stillinger-Weber	bulk Si	32000	11 Mb	4.1x
EIM	crystalline NaCl	32000	14 Mb	6.5x
CHARMM + PPPM	solvated protein	32000	124 Mb	13.6x
MEAM	bulk Ni	32000	54 Mb	15.6x
AIREBO	polyethylene	32640	101 Mb	54.7x
ReaxFF/C	PETN crystal	32480	976 Mb	185x
COMB2 (fixed q) QEq	Ti crystalline SiO_2	32400 32400	31 Mb 85 Mb	55x 284x
eFF	H plasma	32000	365 Mb	306x
ReaxFF	PETN crystal	16240	425 Mb	337x
VASP/small*	water	192 ($512e^-$)	320 procs	17.7×10^6

Intel Xeon 2.66 GHz, single processor

*Not from LAMMPS

Courtesy of Steve Plimpton, Sandia

http://lammps.sandia.gov/bench.html

Example: Mechanical Properties of Metals COMB1

COMB1 potential for Cu/Al

- Single component system (q_i=0)

$$E_T = E_{Tersoff} + E_{bb}$$

Does E_{bb}=0 work for Cu/Al ?

Cohesive energy (eV/atom)	Fcc Cu	Hcp Cu
Expt.	-3.54	(+0.012)
DFT	-3.495	(+0.006)
COMB	-3.54	(+0.0)

With first nearest neighbor shell, fcc and hcp structures can't be distinquished without E_{bb}!

fcc – hcp

TABLE 1 Properties of the first five coordination shells

		Neighbour				
		1st	2nd	3rd	4th	5th
f.c.c.	Number of neighbours	12	6	24	12	24
	Separation/d_0	1	$2^{1/2}$	$3^{1/2}$	$4^{1/2}$	$5^{1/2}$
h.c.p.	Number of neighbours	12	6	2	18	12
	Separation/d_0	1	$2^{1/2}$	$(8/3)^{1/2}$	$3^{1/2}$	$(11/3)^{1/2}$

Applying the potential to 3rd nearest neighbor shell solves the problem, but efficiency is significantly compromised !

E_{bb}: Legendre Polynomial

$$P_0(x) = 1 \qquad P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1) \qquad P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

$$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3) \qquad P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)$$

$$w_i - \sum_{j \neq i} \sum_{k \neq i} f_{C_{ij}} f_{C_{ik}} \left[K^1_{L,P} P^1(\cos\theta_{jik}) + K^3_{L,P} P^3(\cos\theta_{jik}) \right].$$

Bond bending correction

$$E_{bb} = \sum_i \sum_{j \neq i} \sum_{k \neq i} E_{jik} = k \sum_i w_i^{(3)}$$

$$k = (E_{hcp} - E_{fcc}) / 0.833$$

Al: k=0.035/0.833=0.042

Cu: k=0.008/0.833=0.0095

Properties of Al (unpublished)

- Fitted properties

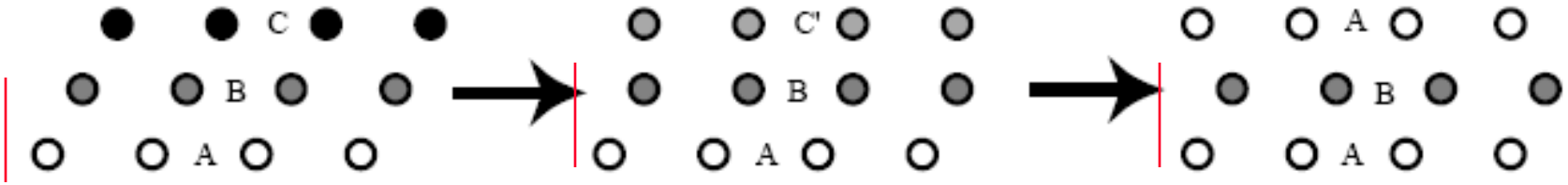
	Exp	DFT	COMB
a_0 (Å)	4.05	4.04	4.047
E_c (eV/atom)	-3.39	-3.40	-3.39
B (GPa)	79	73	72
C_{11} (GPa)	114	113	95
C_{12} (GPa)	62	53	60
C_{44} (GPa)	32	30	35
E (hcp-fcc) (eV/atom)	--	0.035	0.750

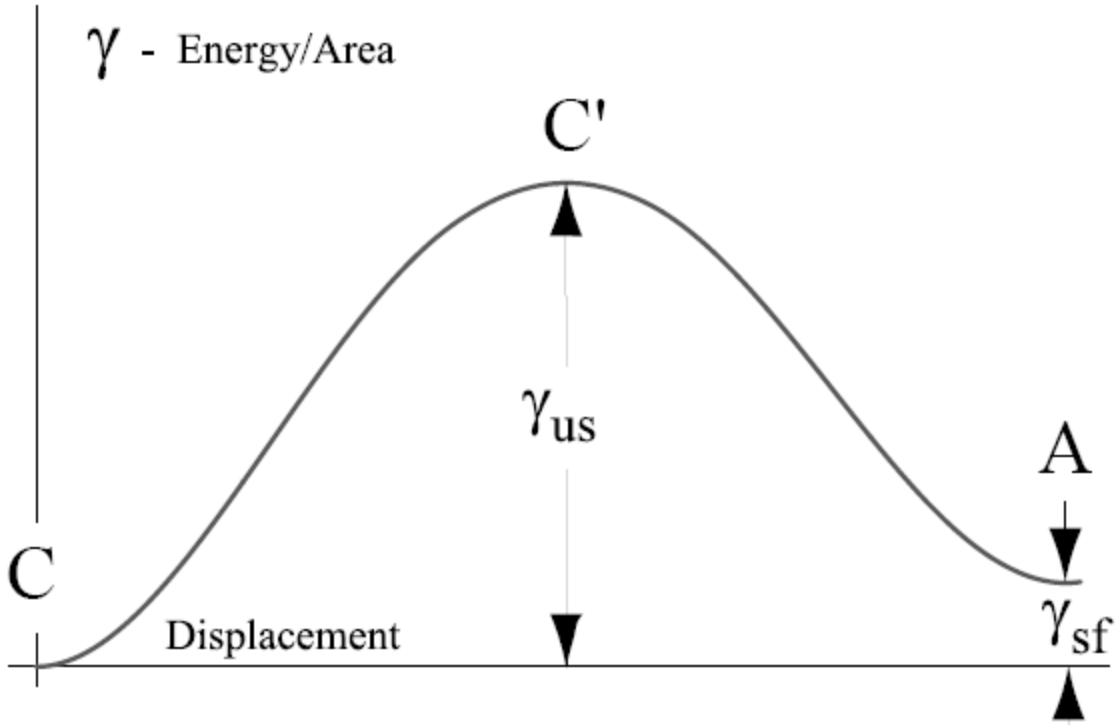
- Predicted properties

	Exp	DFT	COMB
γ (100) (mJ/m^2)	980*	928	1026
γ (110) (mJ/m^2)	980*	992	1193
γ (111) (mJ/m^2)	980*	817	806
E (dia-fcc) (eV/atom)	--	0.750	1.680
Intrinsic SF (mJ/m^2)	--	22	48

Stacking fault energies of fcc metals

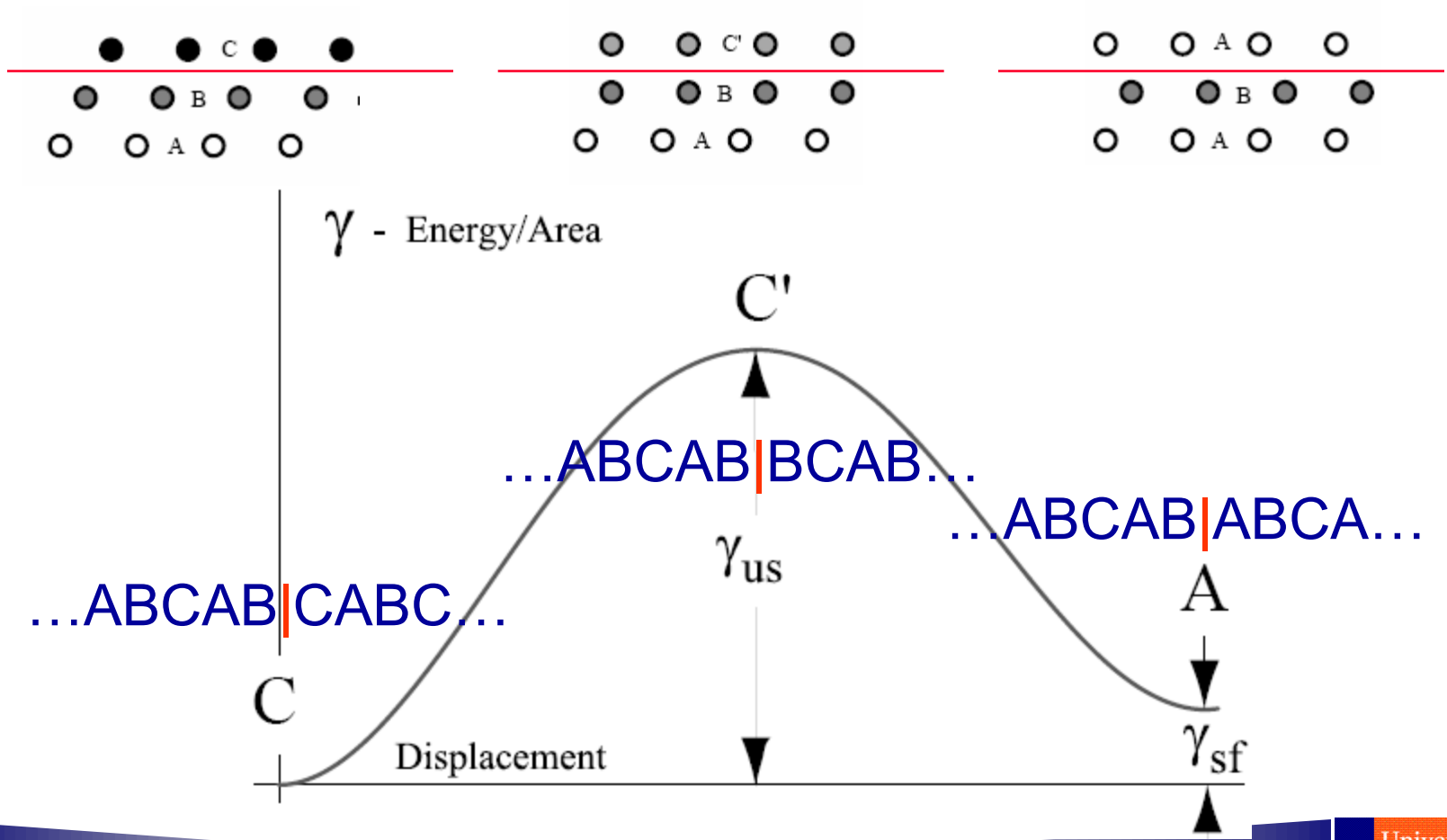
- Stacking fault occurs along <211>



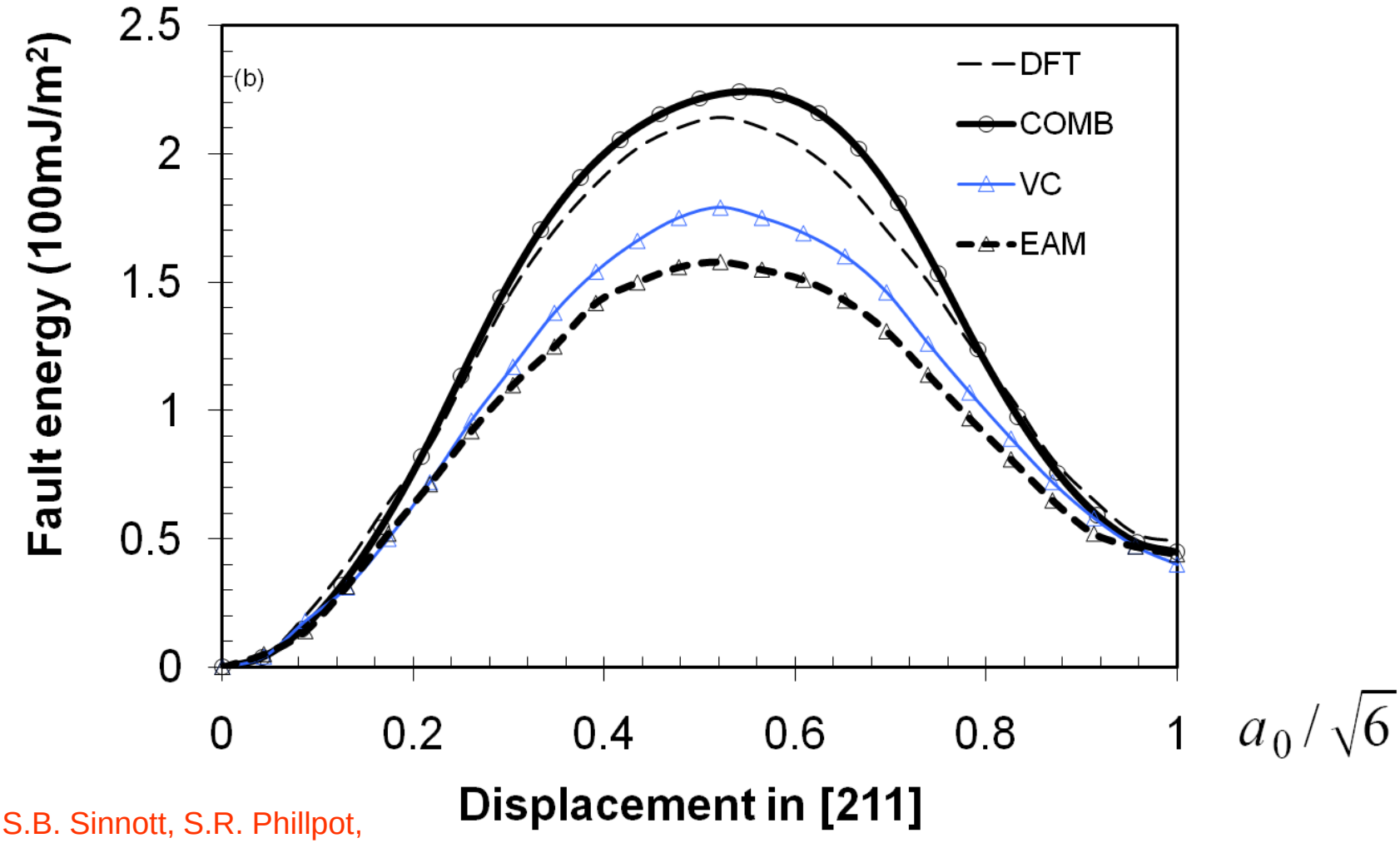


Stacking fault energies of fcc metals

- Displacement along <211>



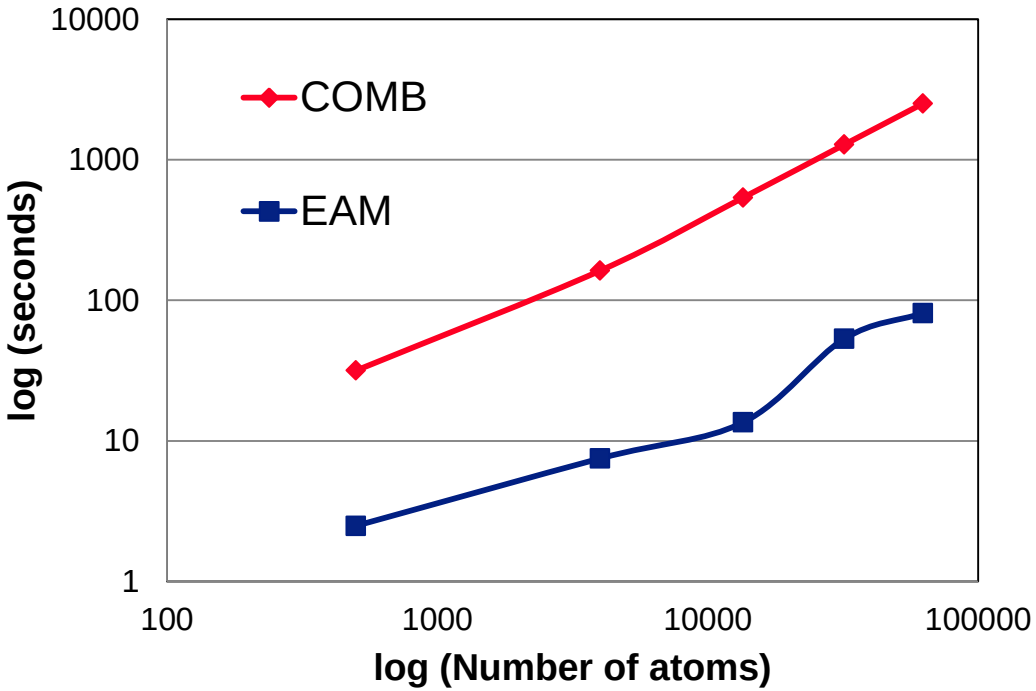
Stacking fault energies – Cu



J. Yu, S.B. Sinnott, S.R. Phillpot, Phil. Mag. Lett. **89**, 136 (2009)

Simulation of a Cu Crystal

- Scaling of COMB1 and EAM in LAMMPS
  - System sizes vary from 500 to 64,000 atoms
  - 8 CPUs, Intel Xeon 2.27 GHz



	EAM [1]	COMB [2]
a_0 (Å)	3.615	3.615
E_{coh} (eV)	-3.54	-3.51
C_{11} (GPa)	170	169
C_{12} (GPa)	123	119
C_{44} (GPa)	76	52
MD Time (seconds. 10^3 atom^{-1}. 10^3 steps^{-1})	2.1	44.8

- COMB1 costs ~25 times more than EAM

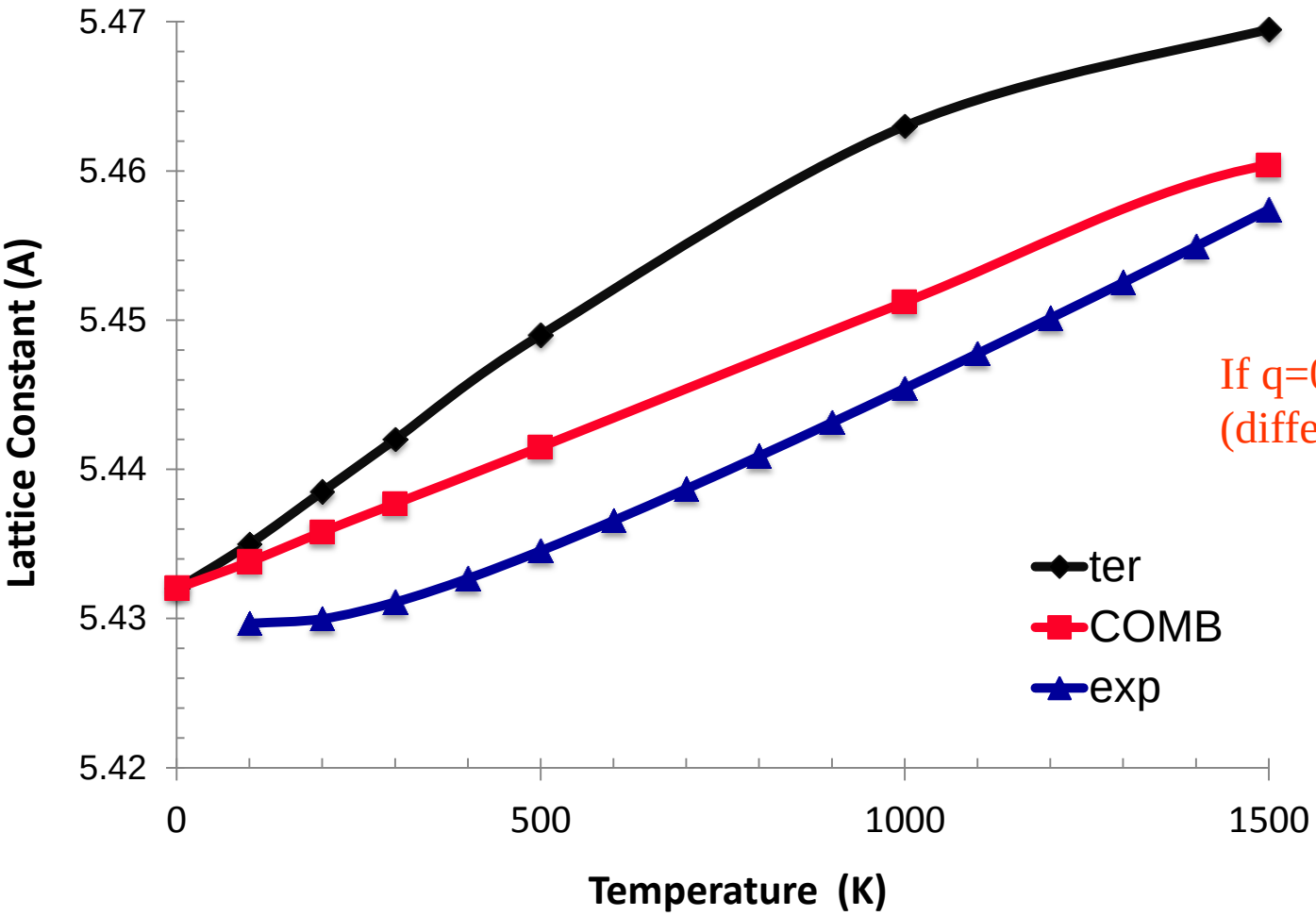
[1] Y. Mishin, JM Mehl, DA Papaconstantopoulos, AF Voter, JD Kress, ***Phys. Rev. B*** 63, 224106 (2001).

[2] J Yu, SR Phillpot, SB Sinnott, ***Phys. Rev. B*** 75, 233203 (2007).

Example: Illustration of Costs and Benefits for Si/SiO_2 COMB2

How does COMB do for Si/SiO_2 ?

- Lattice Constant vs. Temperature for Si



If q=0, COMB~Tersoff
(different parameters)

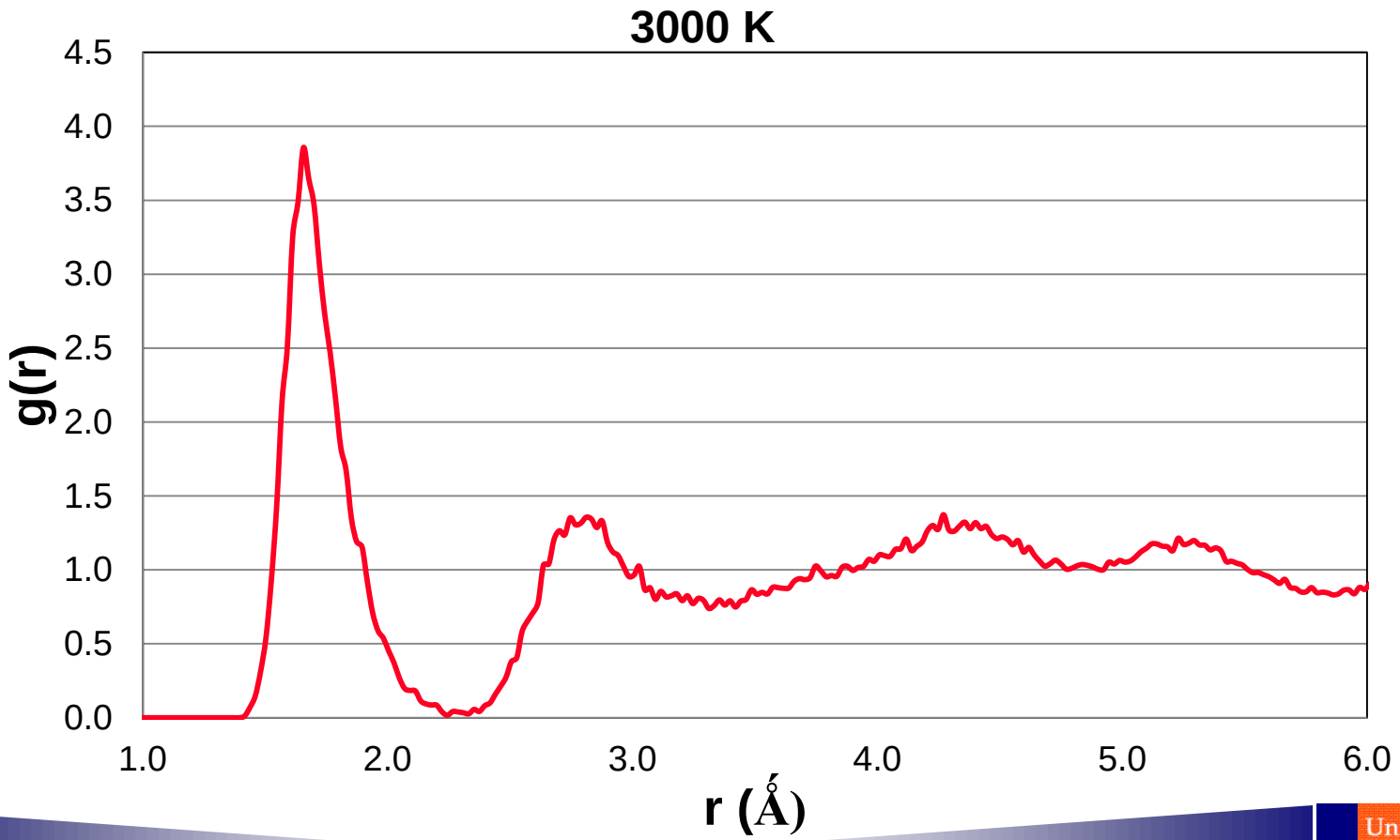
α-Cristobalite surface energies

Surface termination	Surface energy (mJ/m^2)	
	DFT-LDA [a]	COMB
SiO_2(α-C):Si	1795	1491
SiO_2(α-C):O	1185	1073
SiO_2(α-C):OO	917	839

[a] VASP calculations, computational set adapted from "K. **Nagao**, J.B. **Neaton**, N.W. **Ashcroft**, *PRB* 68 125403 (2003)"

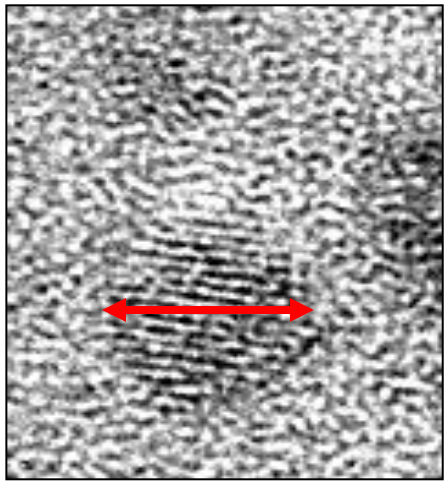
Amorphous SiO_2

- Amorphous silica is the most stable polymorph
  - Most challenging SiO_2 polymorph to model



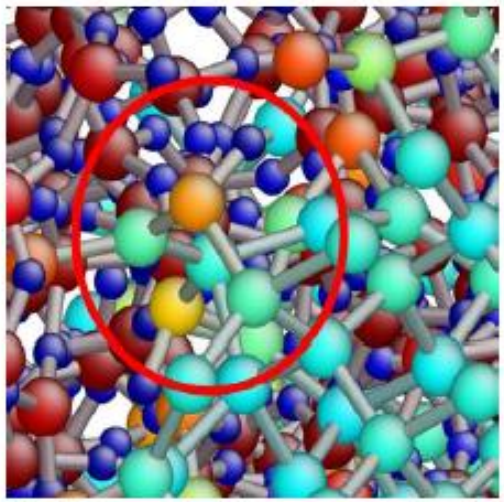
Si Nanocrystals Embedded in a-SiO_2

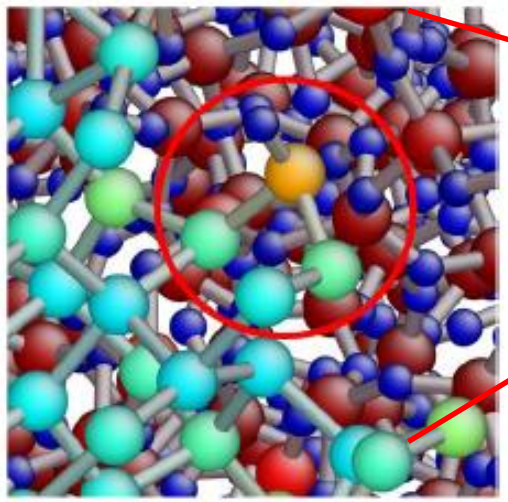
- Si nanocrystals (NCs) emit visible light and the extent of the emission depends on the
  - Size of the Si-NC
  - Structure of the Si-NC/a-SiO_2 interface
    - Silanone bonds (Si=O double bond)

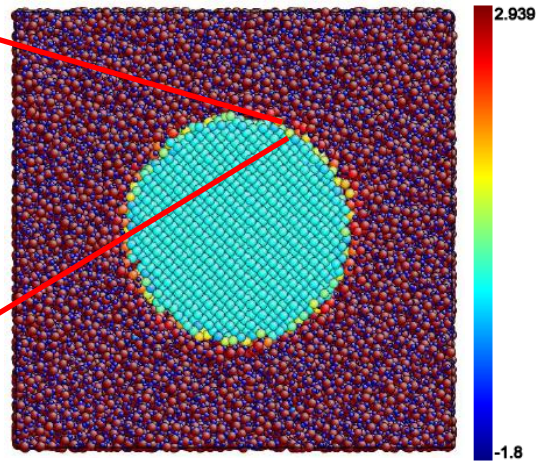


10 nm in diameter

O
Si



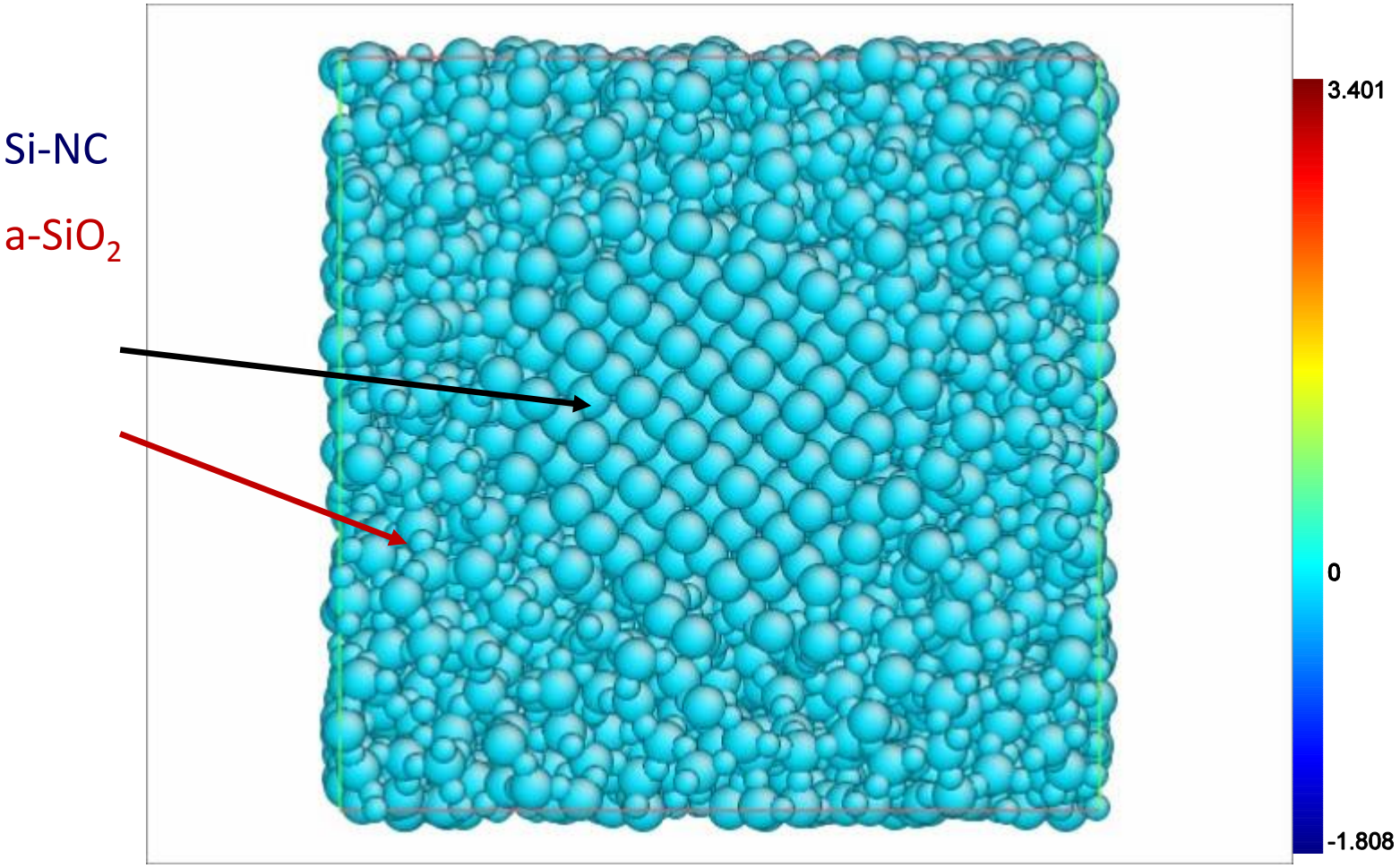




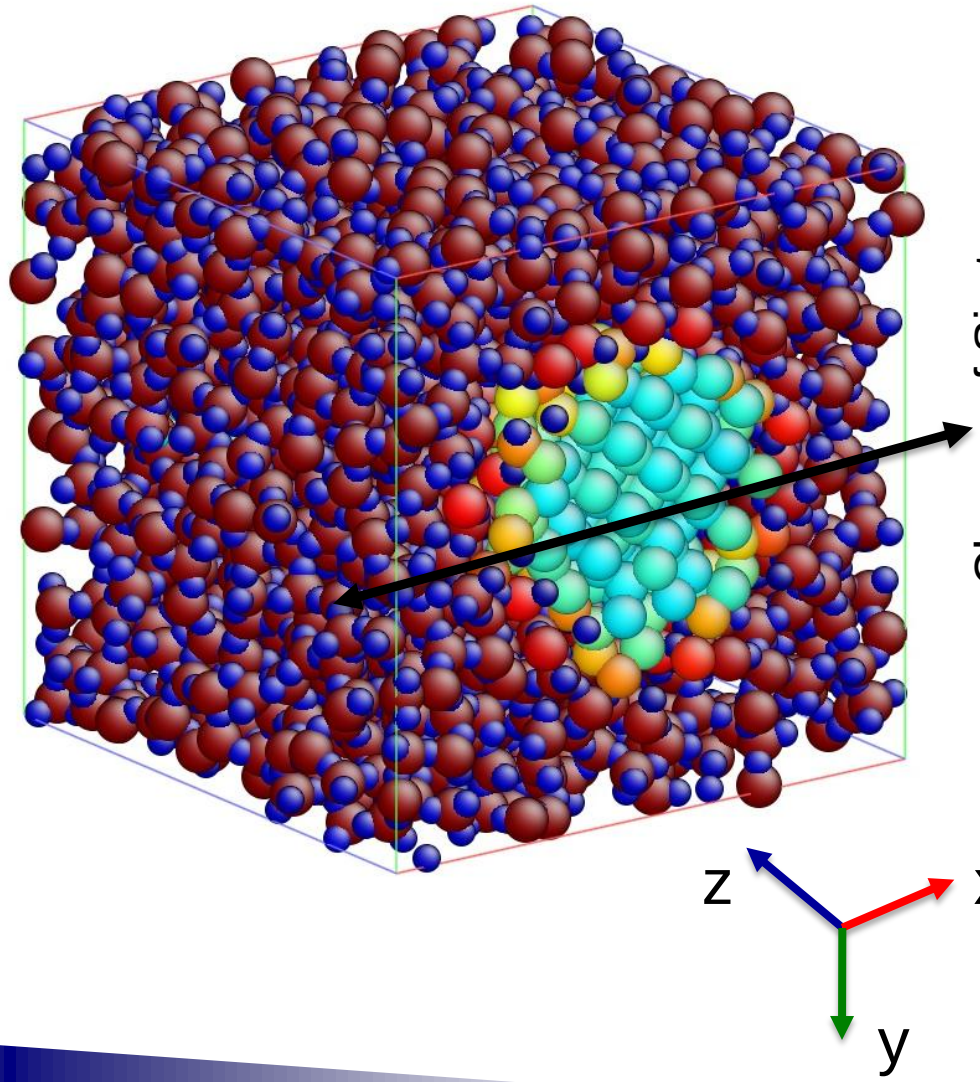
In collaboration with Flyura Djurabekova and Kai Nordlund at the University of Helsinki

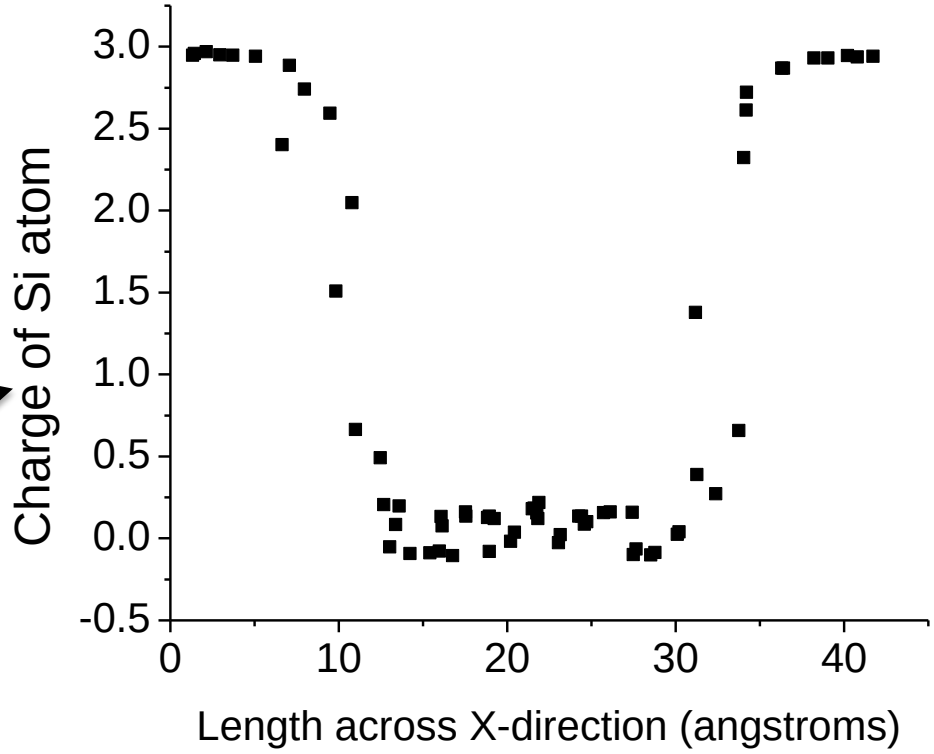
F. Djurabekova, M. Backholm, M. Backman, O. H. Pakarinen, J. Keinonen, K. Nordlund, **T.-R. Shan**, B. D. Devine, and S. B. Sinnott, ***Nucl. Instr. Meth. Phys. Res. B*** 268 19 3095 (2010).

Variable Charge Equilibration



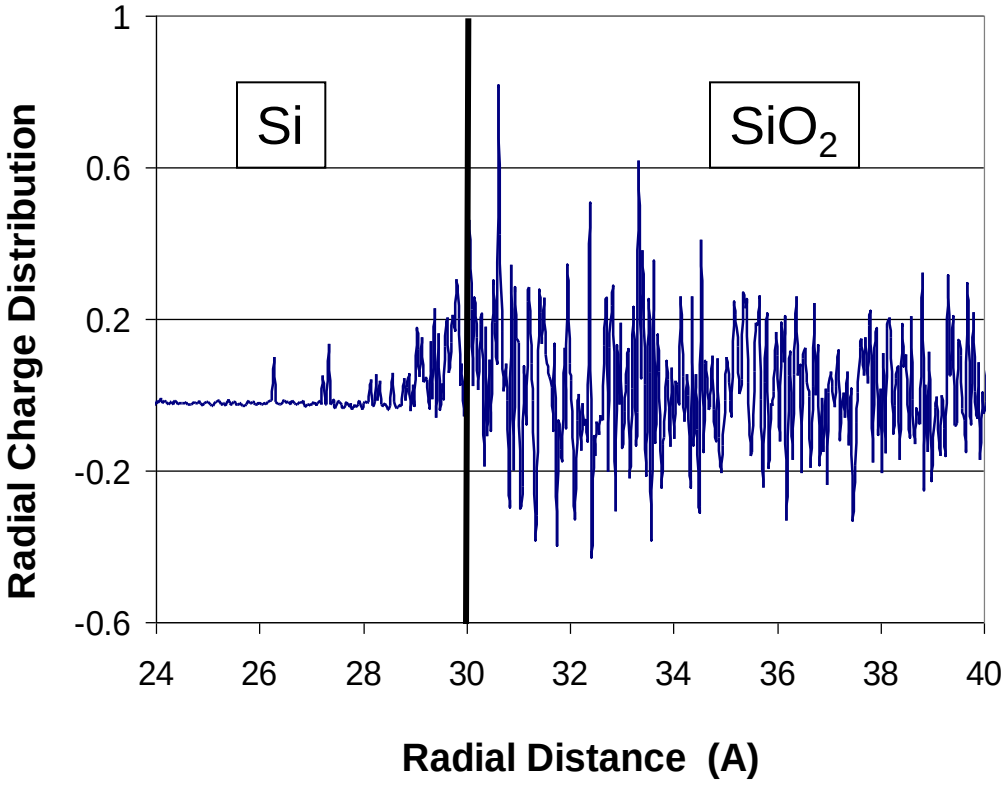
Charge Distribution of a 2 nm NC

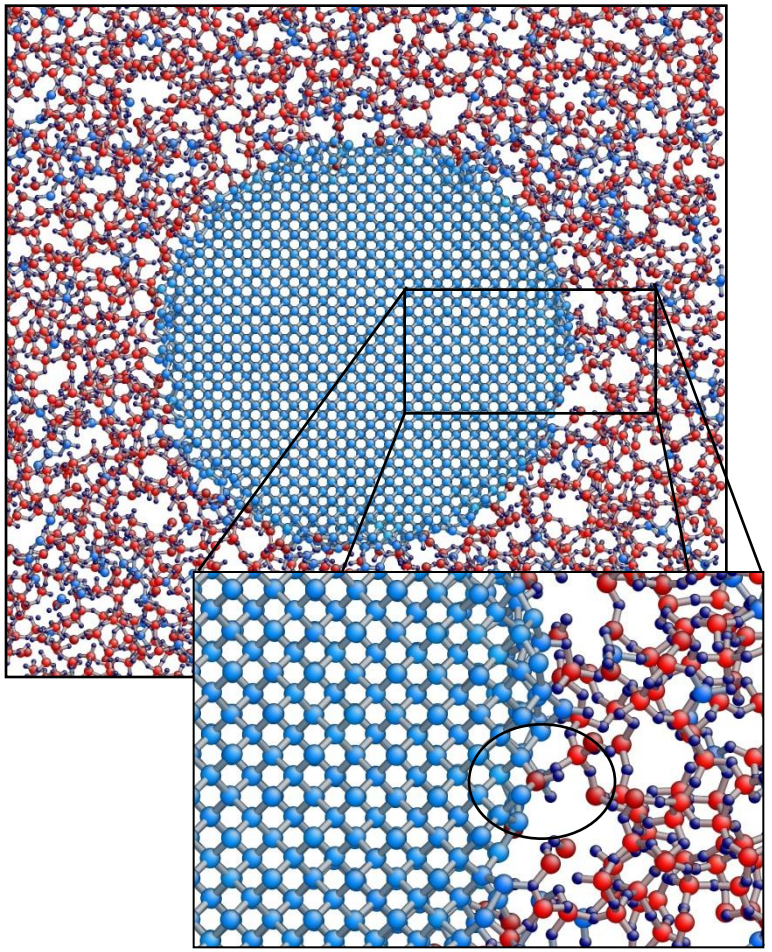




Charge Equilibrated MD of nc-Si/SiO_2

Simulations reveal charge spilling and defects at the interface

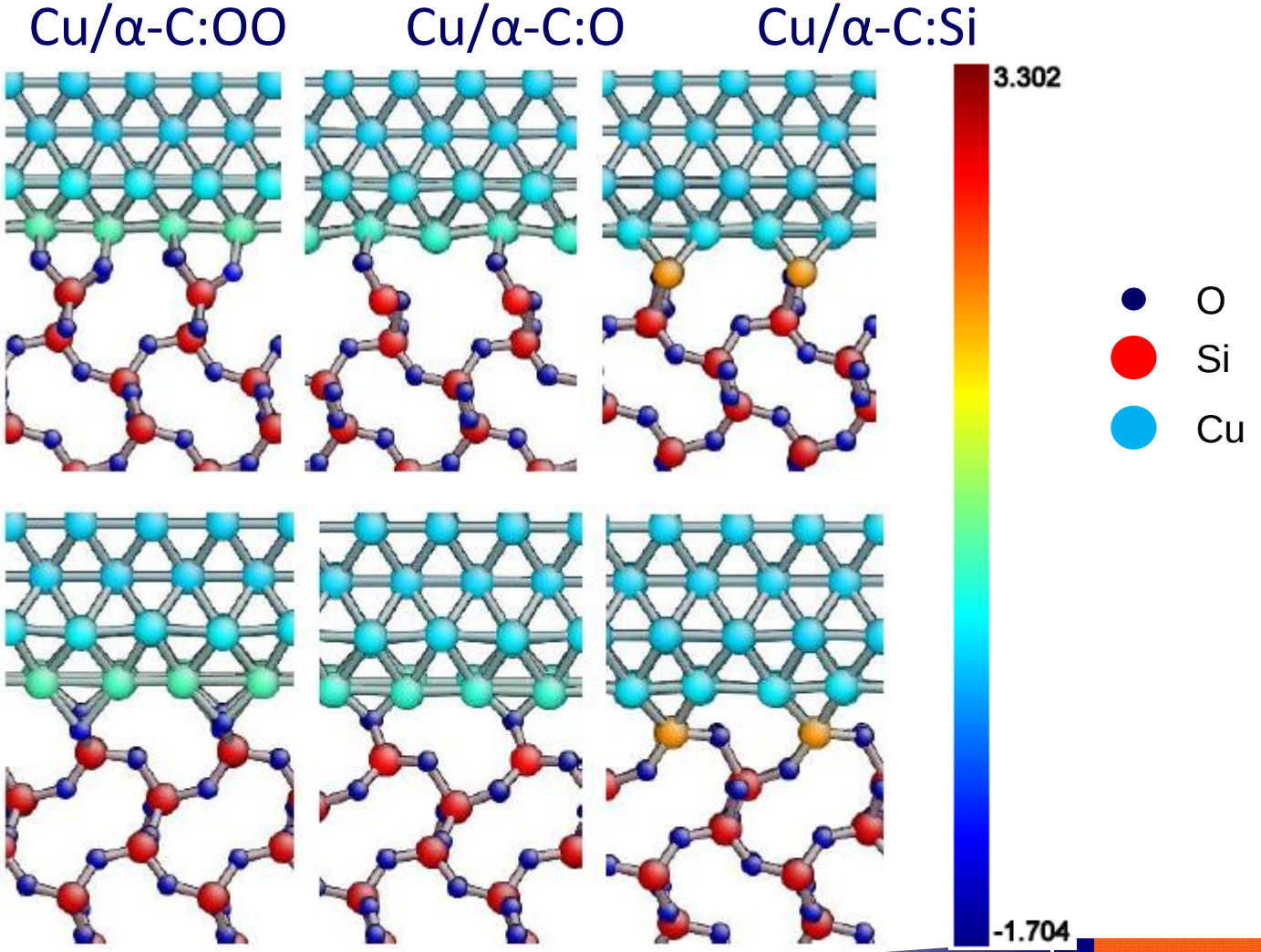




Applications -Heterogeneous Interfacial Structures COMB2

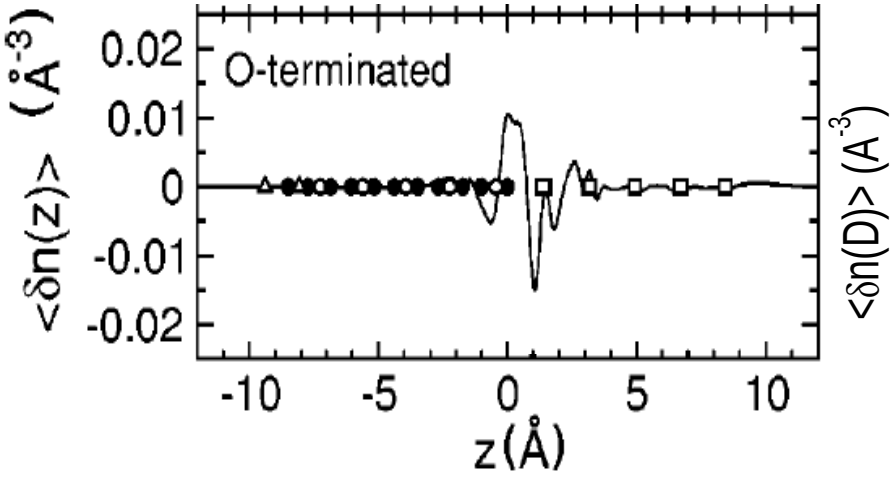
Cu (001)/α-cristobalite (001) Interfaces

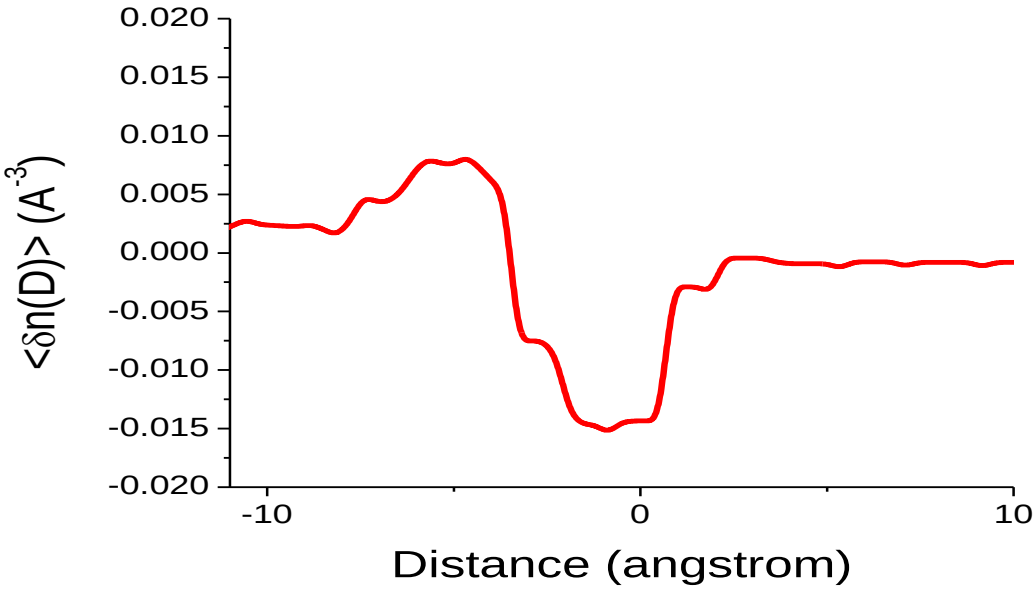
- [100]
- [010]

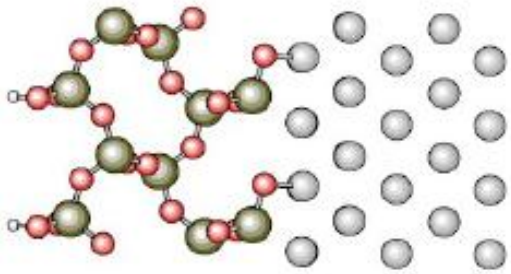


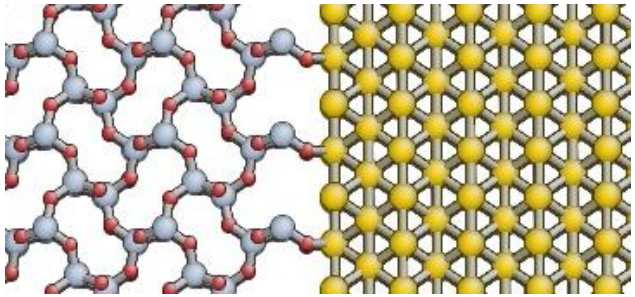
Charge Transfer Across the Interface

- Electron density difference
  - $\langle \delta n(z) \rangle = \langle n_{IF}(z) \rangle - [\langle n_{SiO_2}(z) \rangle + \langle n_{Cu}(z) \rangle]$









Cu (001)/α-cristobalite (001) Interfaces

- Adhesion energy = $(E_{SiO_2} + E_{Cu} - E_{Cu/SiO_2})/A_{IF}$
  - Quantifies the adhesive strength of the interfaces (unit: J/m^2)

Type of interface	DFT-LDA [a]	DFT-LDA [b, c]	DFT-GGA [c]	COMB [c]
Cu/α-C:Si	1.406	1.432	1.034	0.864
Cu/α-C:O	1.555	1.591	1.222	1.734
Cu/α-C:OO	3.805	3.987	3.601	3.591

Expt. ~ 4 J/m^2

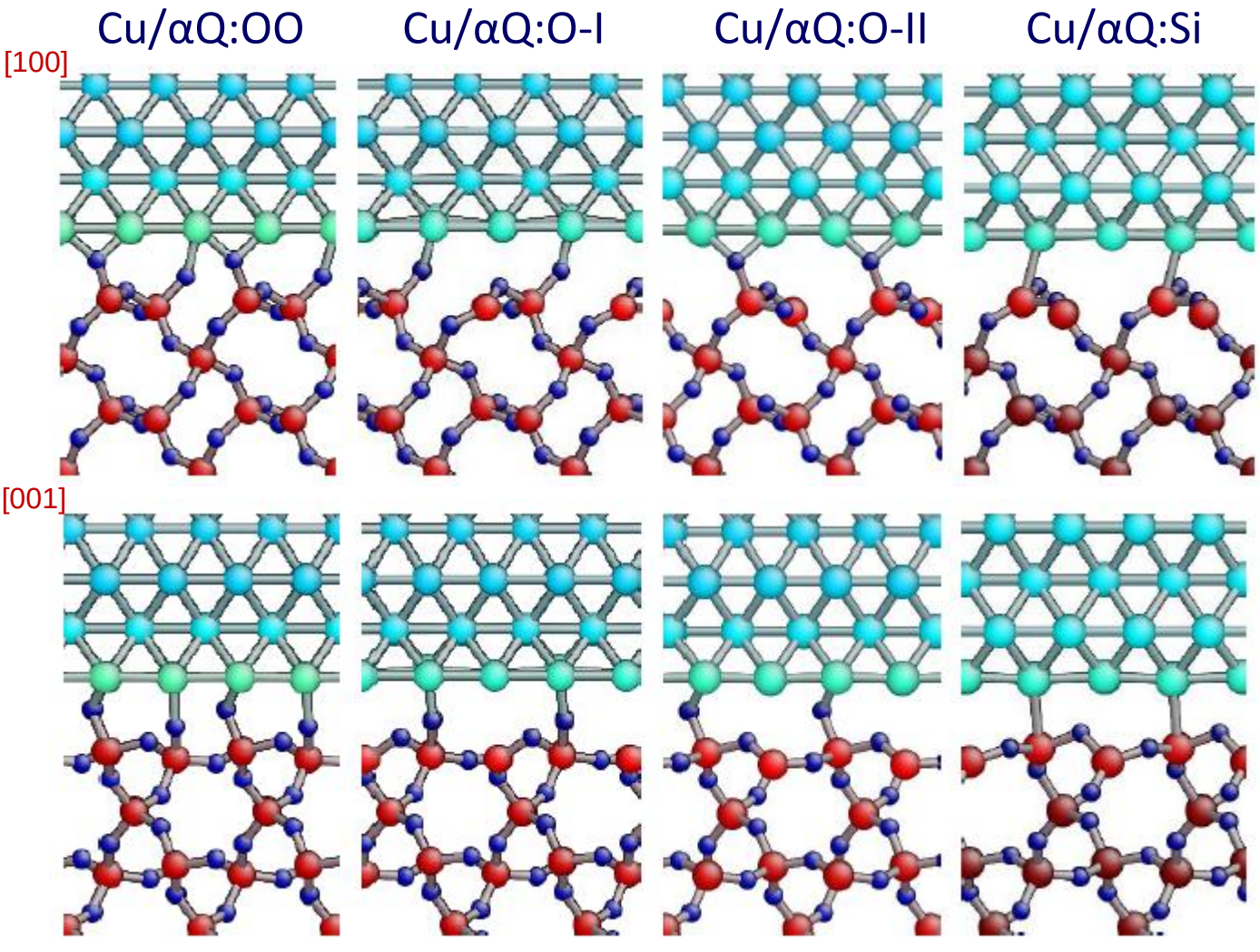
- Average interfacial bond lengths

	DFT-LDA	DFT-GGA	COMB
Cu-O	1.90 Å	1.93 Å	1.86 Å
Cu-Si	2.40 Å	2.47 Å	2.32 Å

COMB potential reproduces structural and adhesive properties of Cu/αC

[a] K. Nagao, J.B. Neaton, N.W. Ashcroft, ***Phys. Rev. B*** 68 125403 (2003)
[b] VASP calculations with computation details adapted from Ref [a], except US for Si
[c] **T.-R. Shan**, B. D. Devine, S. Phillpot, S. Sinnott, ***Phys. Rev. B*** *83 115327* (2011)

Cu (001)/α-quartz (010) Interfaces



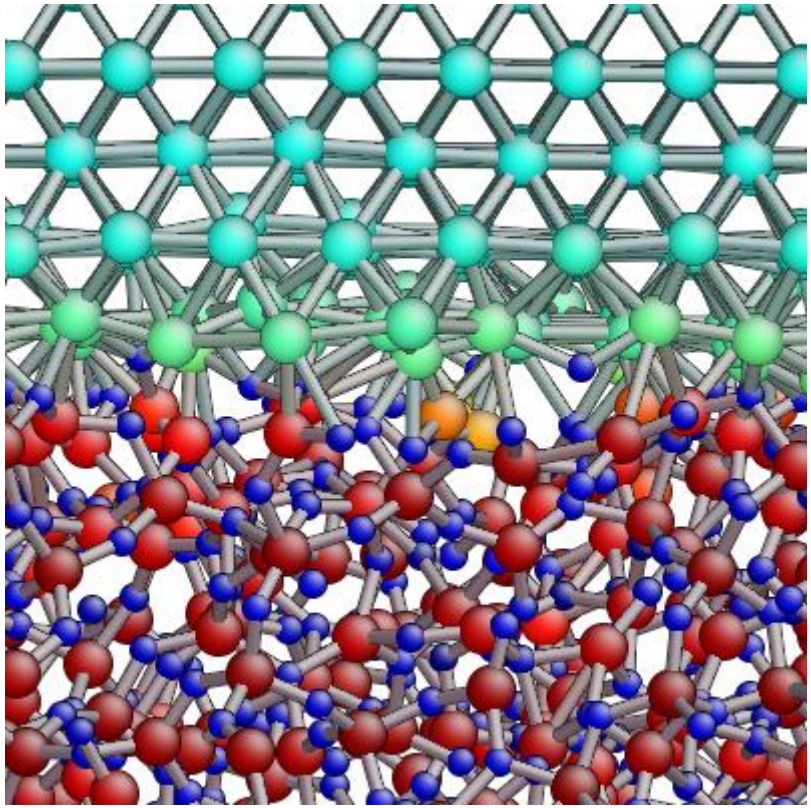
COMB potentials

Type of interface	W (J/m^2)
Cu/α-Q:Si	0.850
Cu/α-Q:O I	2.494
Cu/α-Q:O II	2.646
Cu/α-Q:OO	3.472

O
Si
Cu

Cu (001)/a-SiO_2 Interfaces

- Structural properties of the interface
  - Oxidation of Cu is limited to the first two Cu layers; formation of Cu_2O



- Introduced O vacancies at the interface
  - 0, 10 and 20 V_O

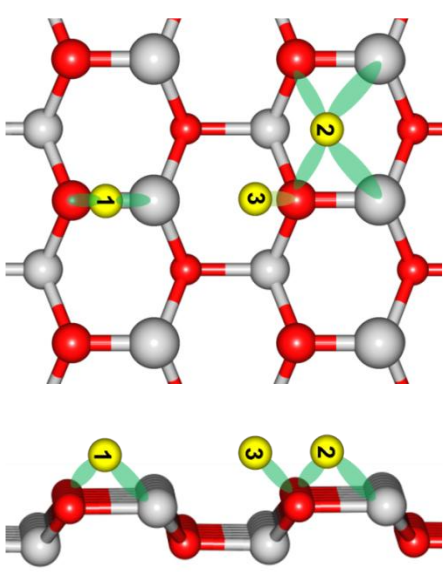
Type of interface	W (J/m^2)		Cu-O (%)
	Exp	COMB	
Cu/a-SiO_2 + 0 V_O	0.5 - 1.2 [a] 0.6 - 1.4 [b]	1.810	22
Cu/a-SiO_2 + 10 V_O		0.629	13
Cu/a-SiO_2 + 20 V_O		0.289	11

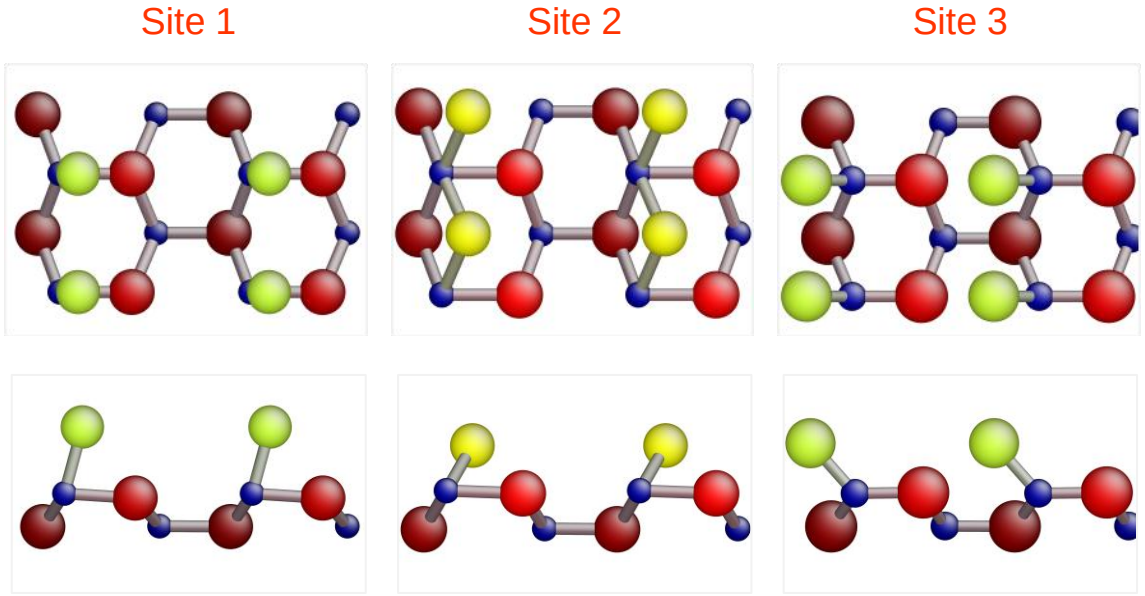
- Cu-O bonds play crucial roles in adhesion of the interface
- Adhesion of Cu/dielectric layer decreases with O defects

[a] T. S. Oh, R. M. Cannon, and R. O. Ritchie, ***J. Am. Ceram. Soc***. 70, C352 (1987).
[b] M. Z. Pang and S. P. Baker, ***J. Mater. Res***. 20, 2420 (2005).

Applications
-Atoms and Clusters on Surfaces
COMB3

Adsorption of Cu adatom on ZnO($10\bar{1}0$)





$$E_{ads} = E_{ZnO} + E_{Cu} - E_{Cu/ZnO}$$

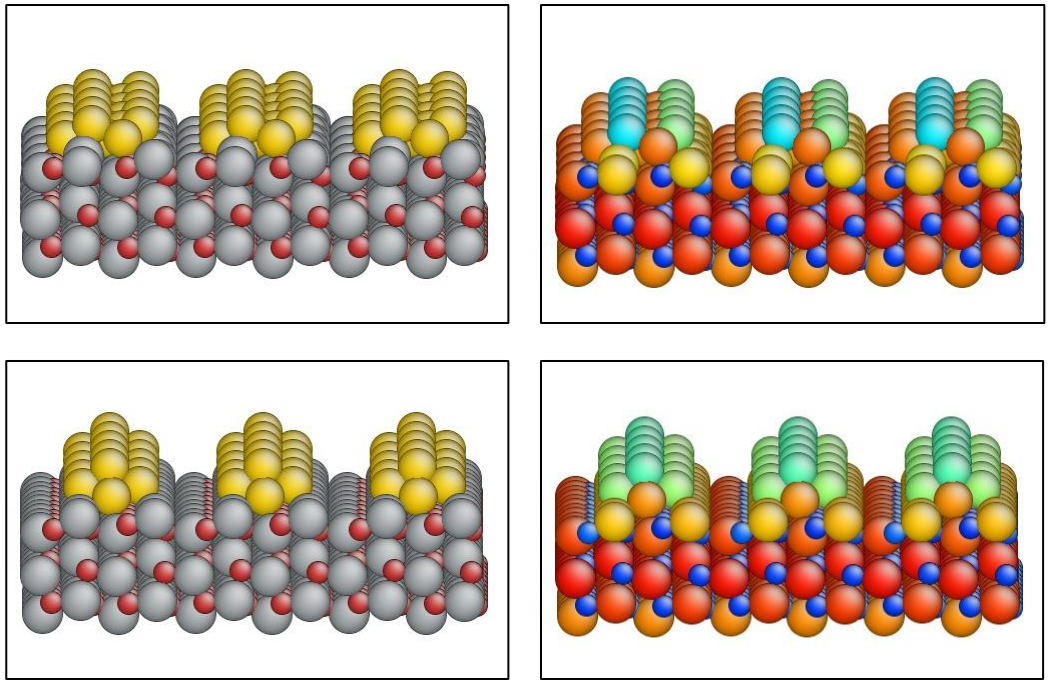
Adsorption E (eV)	Site 1	Site 2	Site 3
DFT-PBE	1.81	1.88	2.09
COMB	1.87 (+3.3%)	1.92 (+2.1%)	1.96 (-6.2%)

Cu_X Clusters on the $ZnO(10\bar{1}0)$ Surface

X=5

planar

stack

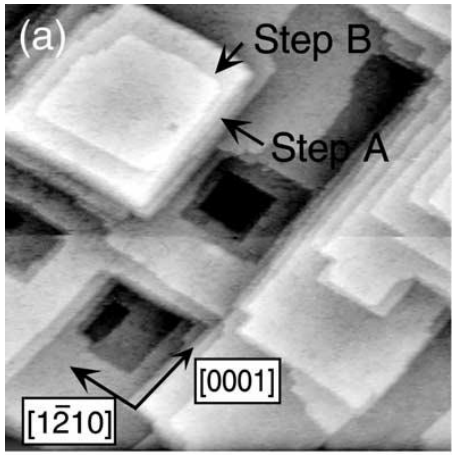


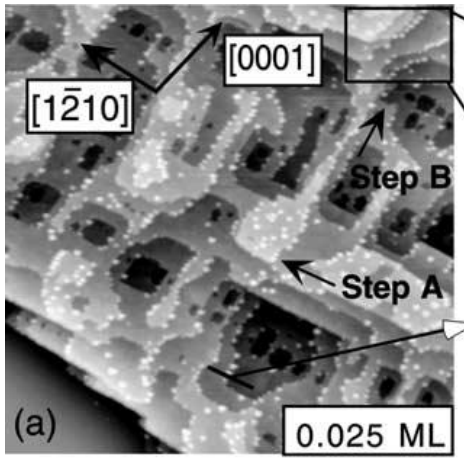
Binding energy (eV)

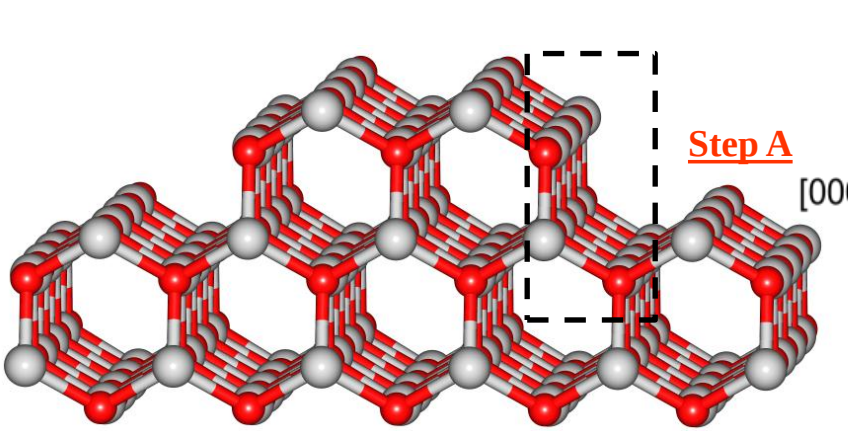
	X=3		X=4		X=5	
	Row	Stack	Flat	Stack	Planar	Stack
DFT	-2.33	-2.37	-2.28	-2.33	-2.31	-2.35
COMB	-3.40	-3.46	-3.24	-3.89	-3.17	-3.59

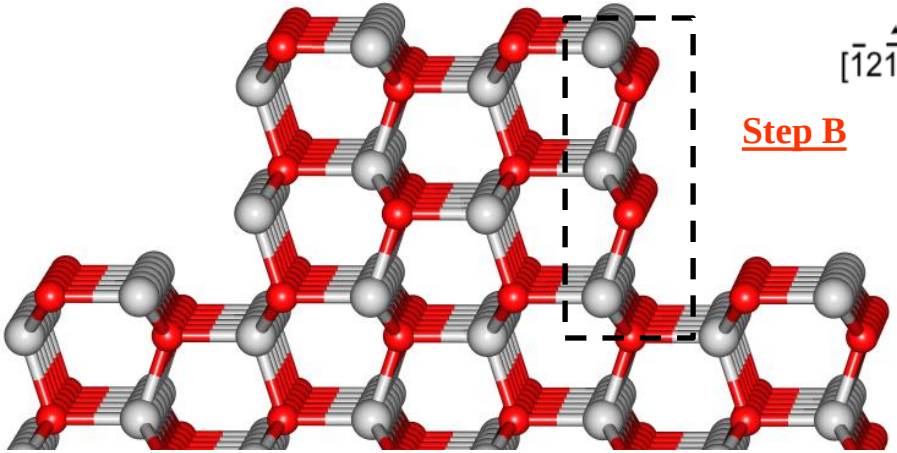
**DFT results courtesy of Xiaowa Nie, Ohio State*

Growth of Cu clusters on ZnO surfaces



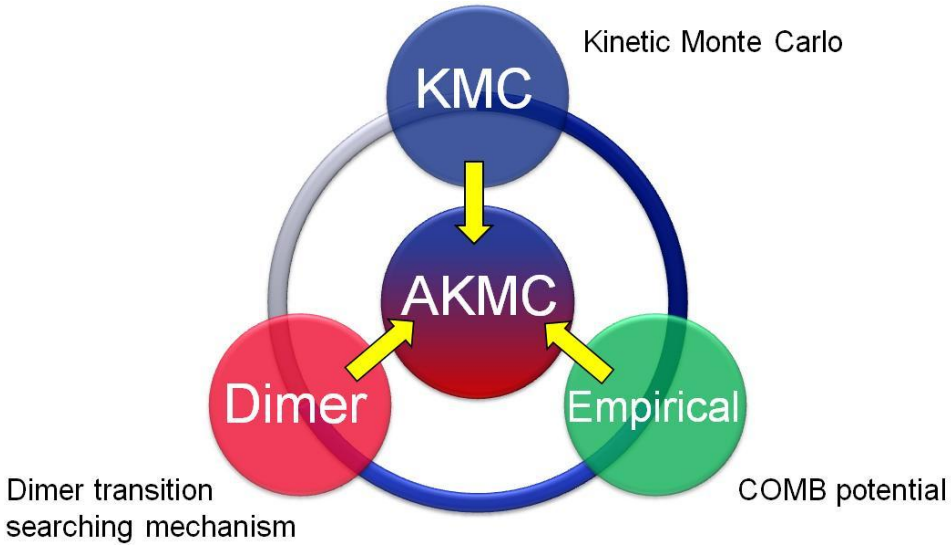






O. Dulub, L. A. Boatner, U. Diebold, Surface Science 504 (2002) 271

Adaptive kinetic Monte Carlo

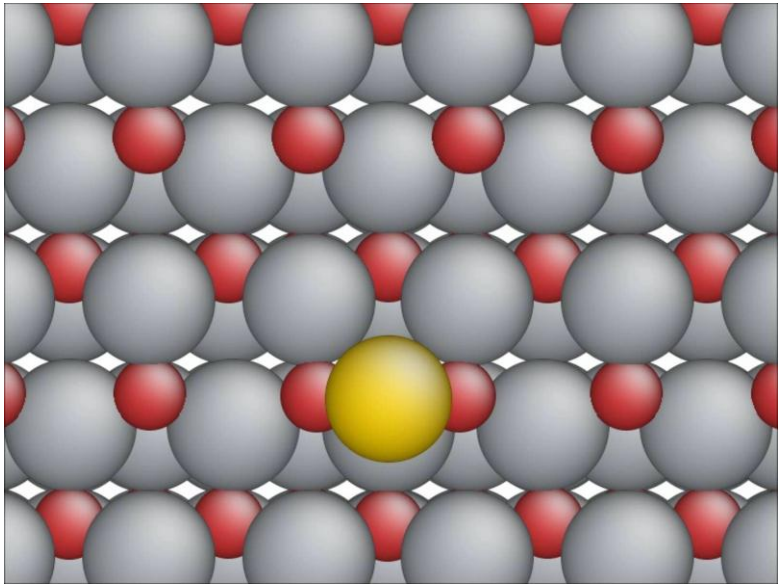


Standard KMC

1. Find low energy saddle point using the dimer method[1,2].
2. The rate of each transition path is calculated using HTST. ($r_i = \nu_0 e^{-\Delta E / k_B T}$)
3. Hop to the final state of the chosen process. ($p_i \propto r_i$)
4. Increment time by an average amount Δt. ($\Delta t = -\ln u / \sum r_i$)
5. Repeat from step 1

Dimer method (transition searching):

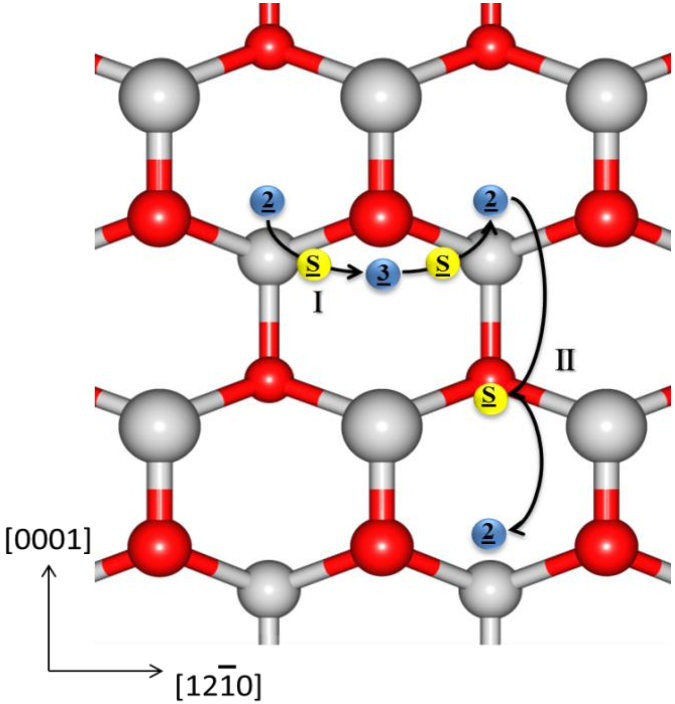
Using the first derivative of the potential energy and the initial state of the transition to find saddle points.

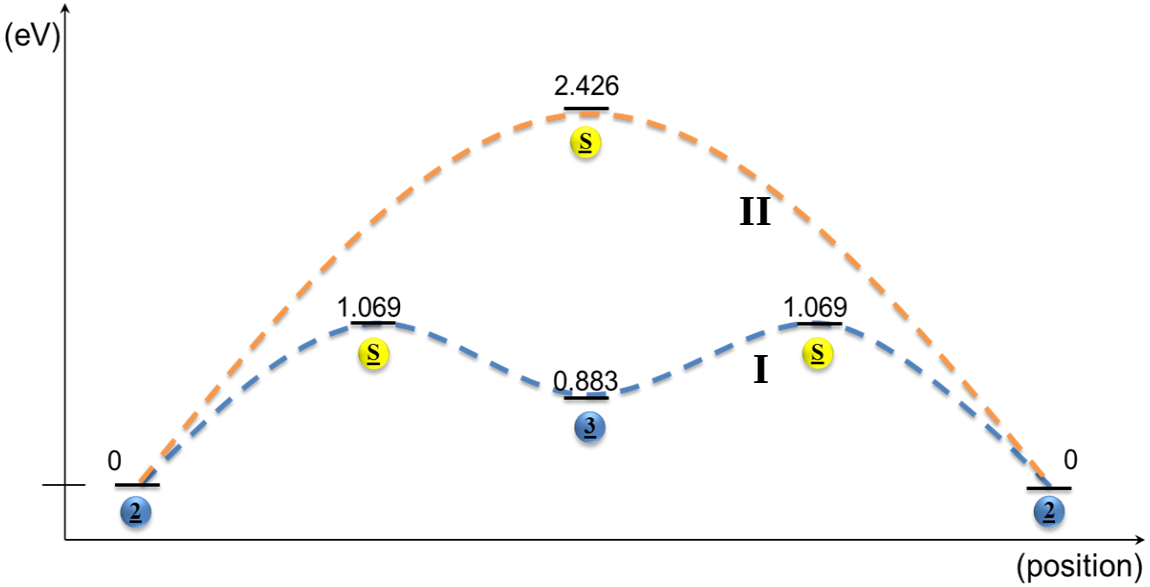


1. G. Henkelman and H. Jonsson, ***J. Chem. Phys.* 111**, 7010 (1999)
2. G. Henkelman and H. Jonsson, ***J. Chem. Phys.* 115**, 9657 (2001)

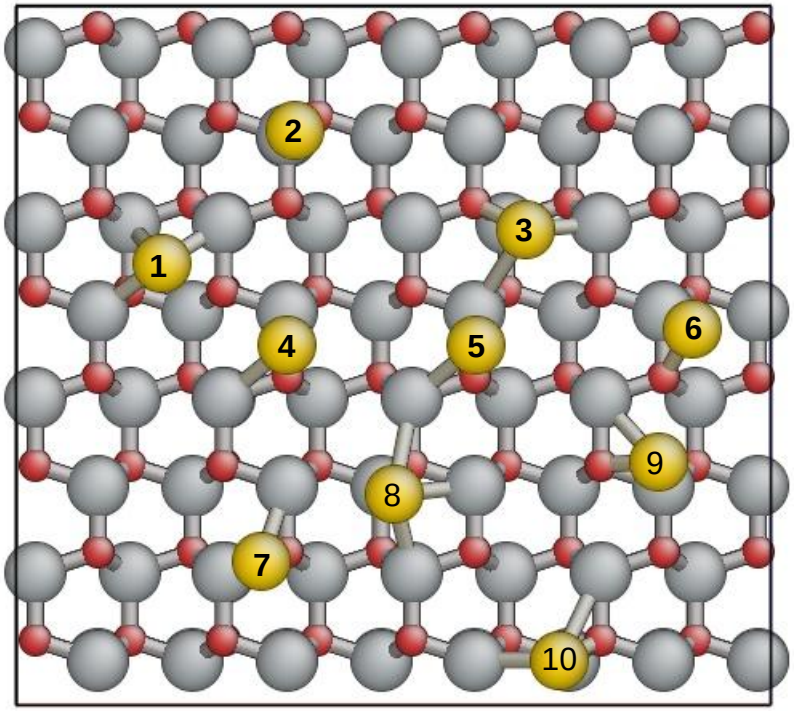
Migration barriers of Cu on ZnO(10$\bar{1}$0)

Cu atom migration along [12$\bar{1}$0] is much easier than along [0001]

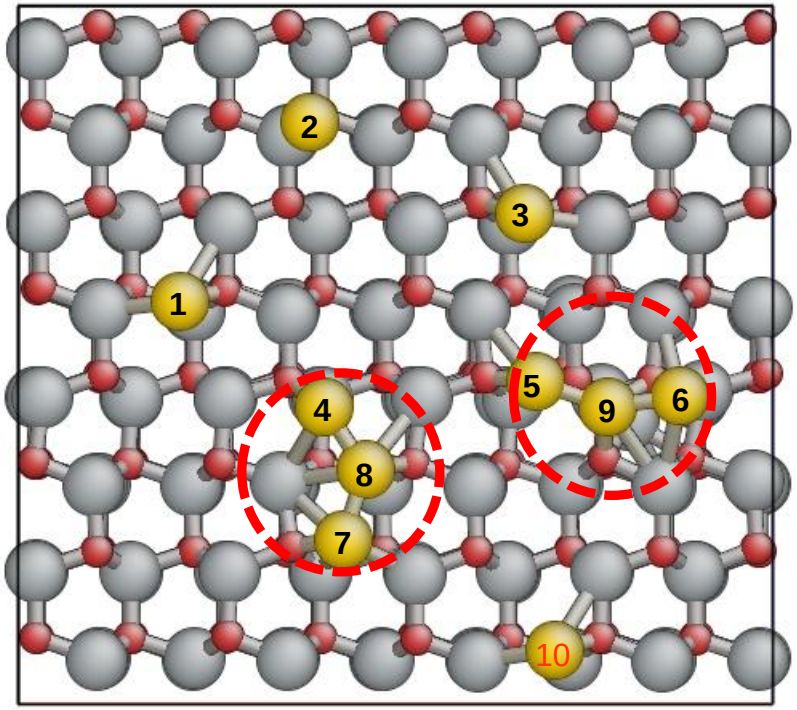




AKMC: Aggregation of Cu atoms on ZnO(10$\bar{1}$0)



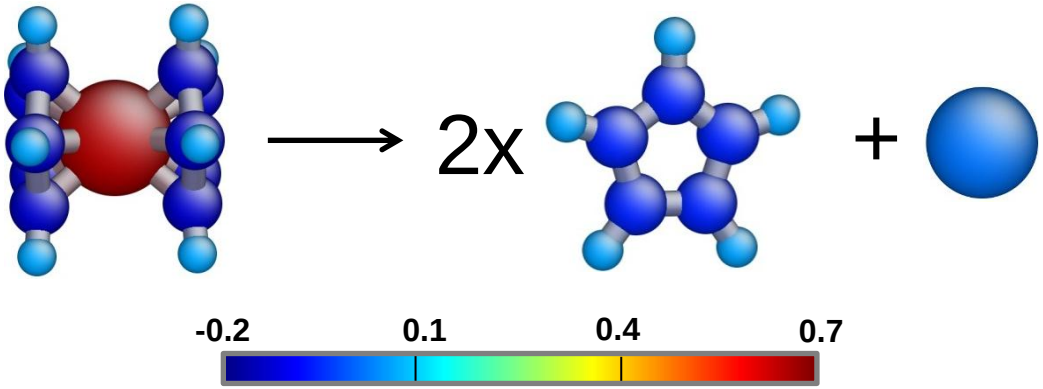
Initial structure
T = 0 ns



After 15 AKMC runs
T = 5 ns

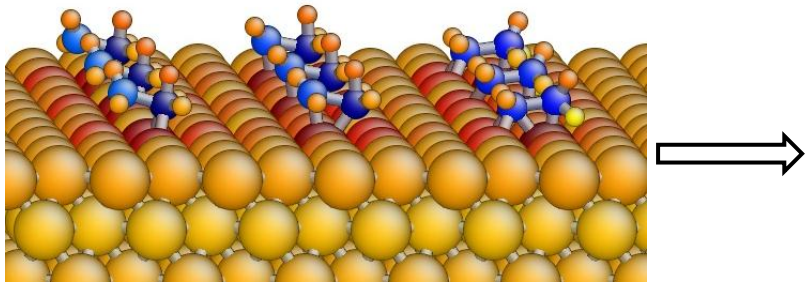
Applications
-Surface Chemistry
COMB3

Properties of COMB Potentials - C/H/Cu



Target (kcal mol^{-1})	COMB (kcal mol^{-1})
122	122

Cu metallocene dissociation

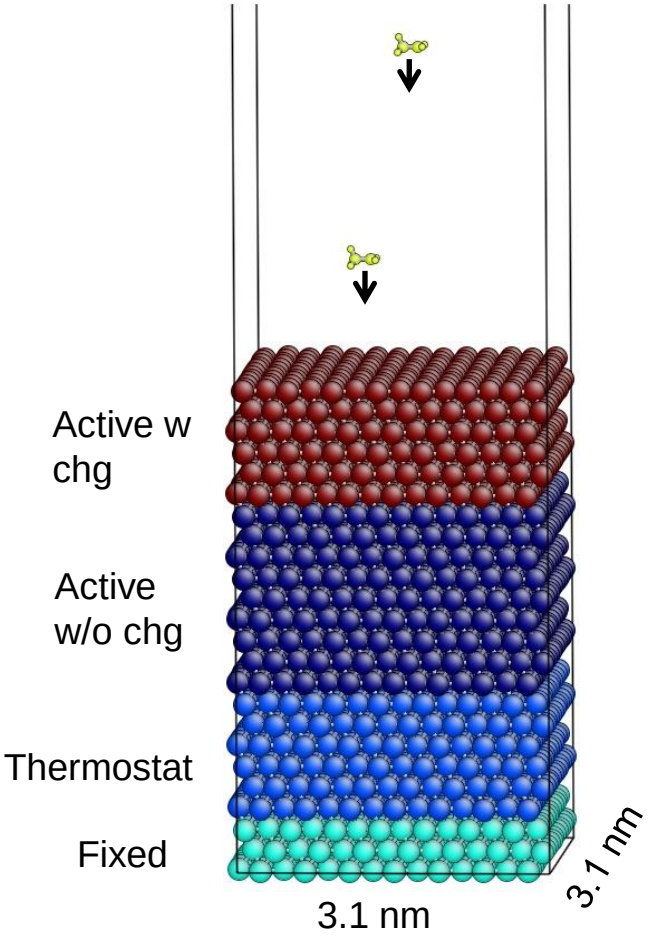


Surfaces	DFT (kcal mol^{-1})	COMB (kcal mol^{-1})
Cu (100)	-36.2	-46.6 to -24.3
Cu (110)	-39.9	-49.5 to -27.1
Cu (111)	-30.9	-45.3 to -19.7

Ethyl adsorption on Cu surfaces

Xin Li et al., J Chem Phys 127, 144710 (2007)

CH_3CH_2 Deposition on the Cu (111) Surface

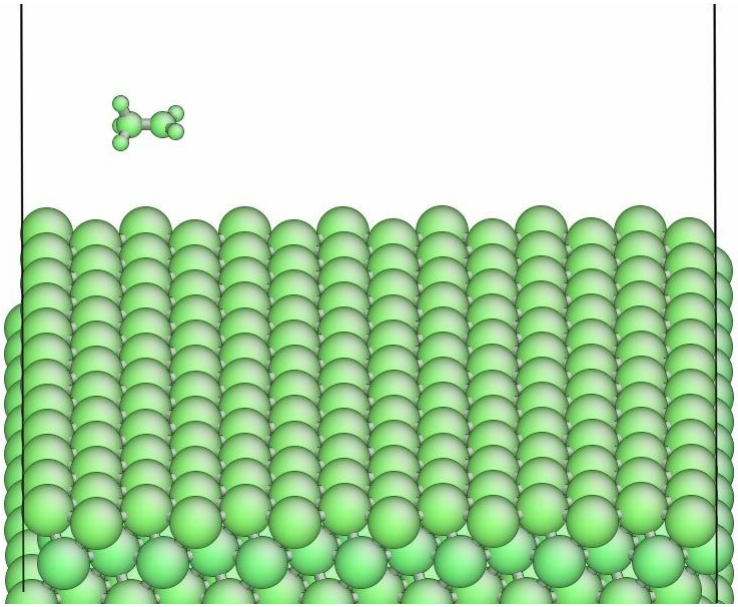


Summary:

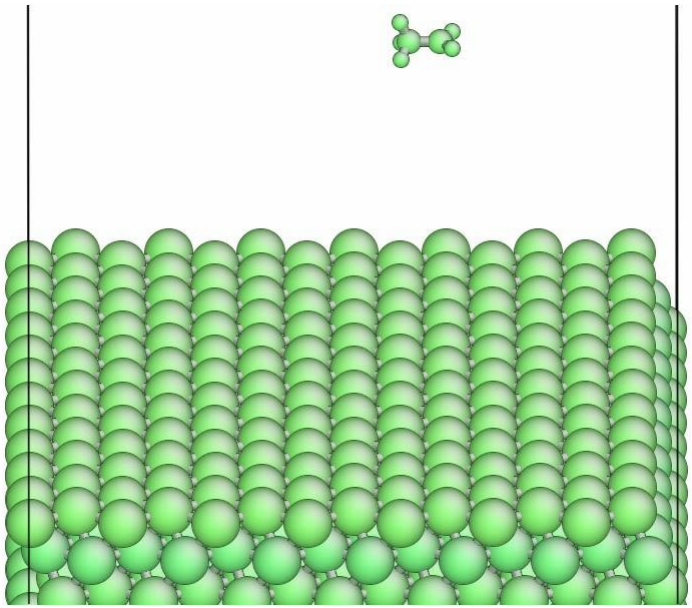
- 12 CH_3CH_2 molecules deposition on Cu(111) surface
- Two incident energy levels
  - 5 eV mol^{-1}
  - 10 eV mol^{-1}
- Molecules are randomly distributed
- The relaxation time between two molecules is 0.5 ps
- Temperature is set to 300K

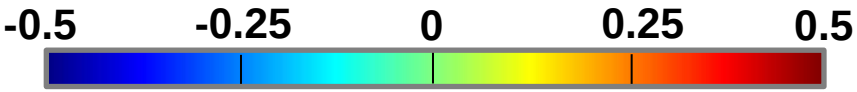
CH_3CH_2 Deposition on the Cu (111) Surface

5 eV

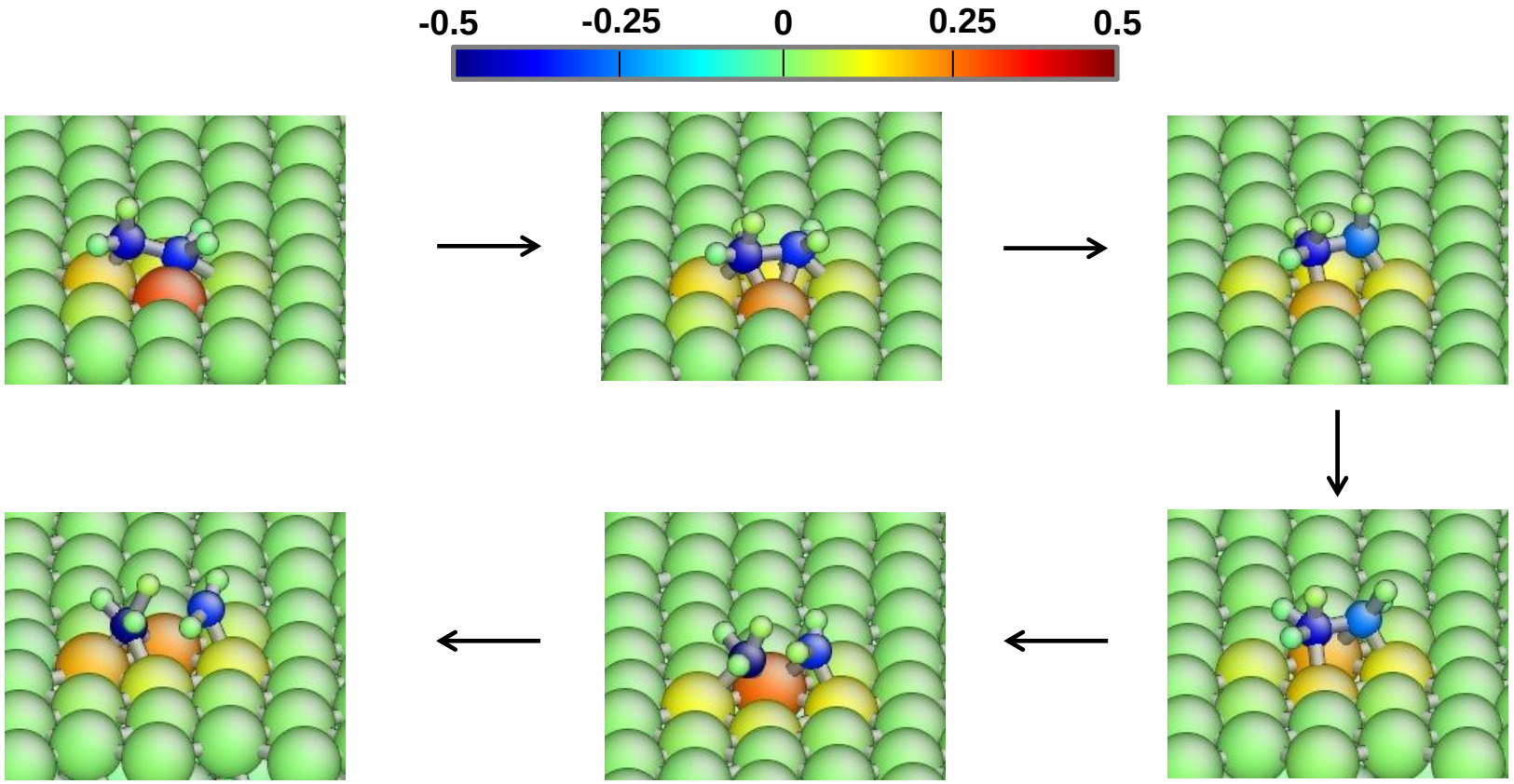


10 eV

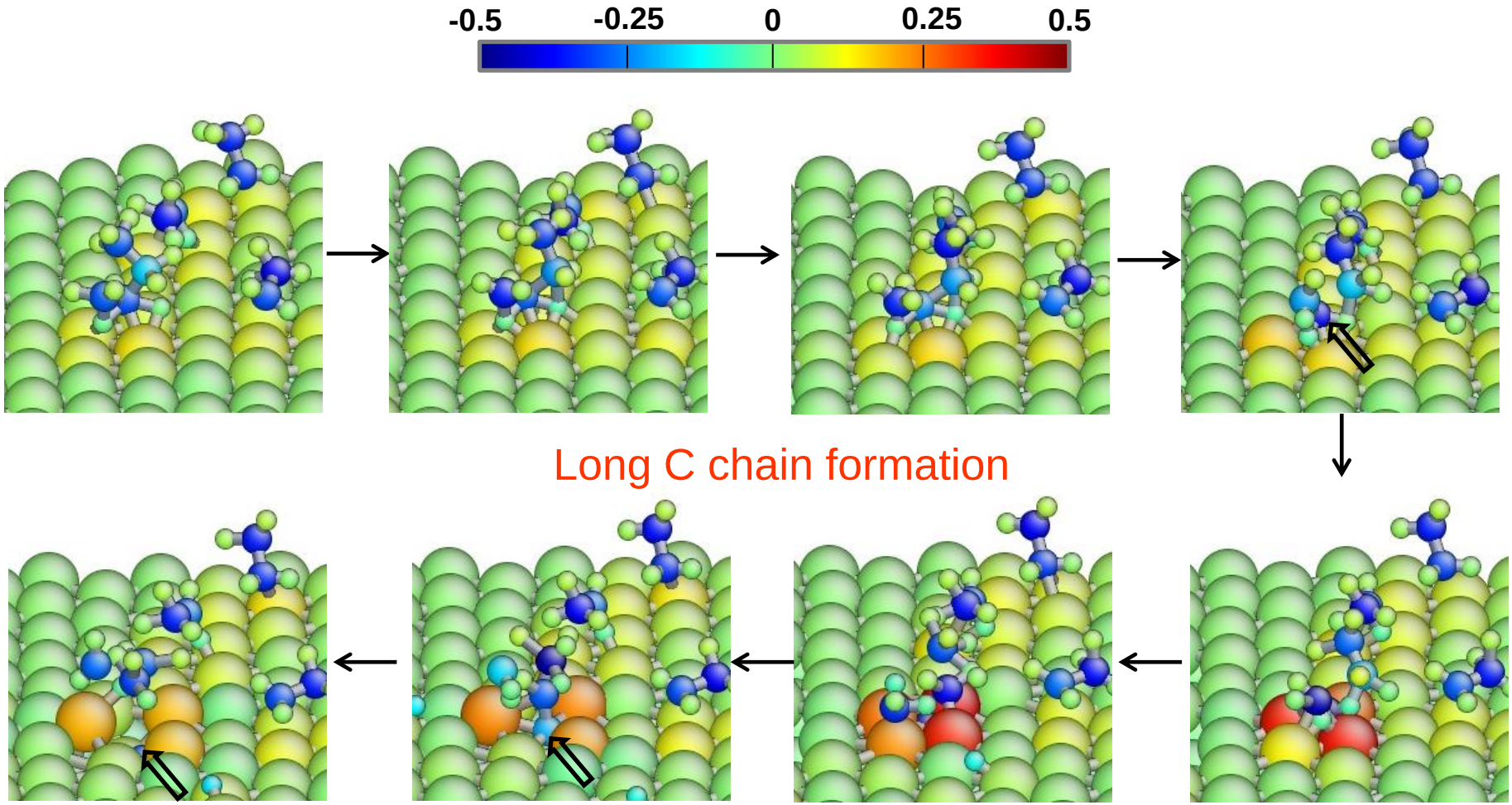




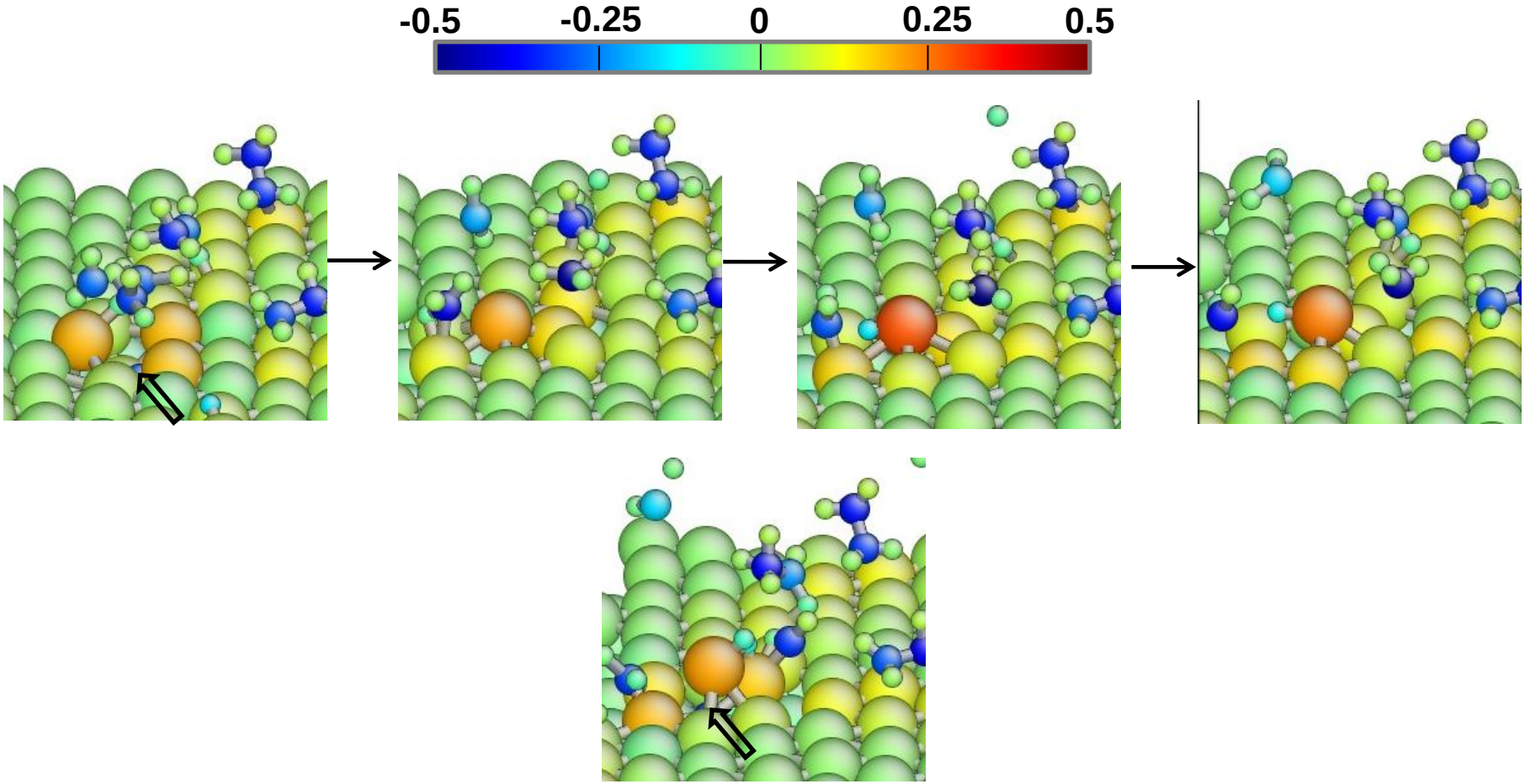
Dissociation of CH_3-CH_2



Collision-Induced Dissociation Reactions



Displacement of Surface Atoms

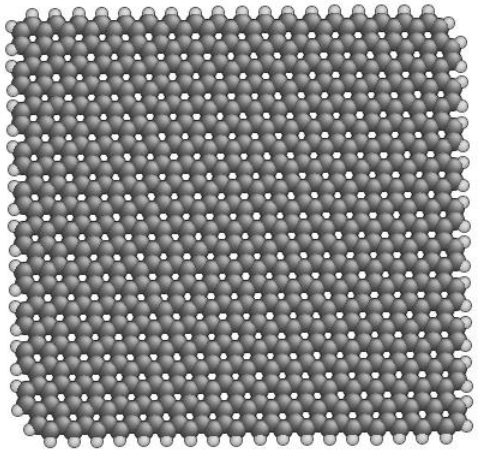


Cu^{ko} formation

Applications
-Graphene Adhesion to Cu_2O
COMB3

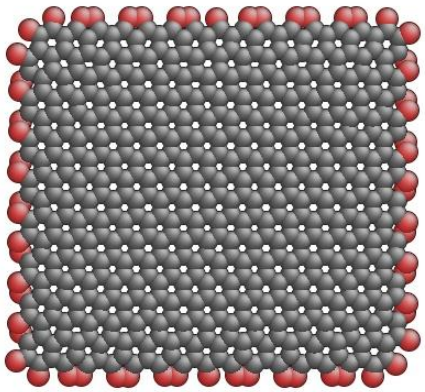
Graphene Adhesion on Cu_2O

796 C atoms



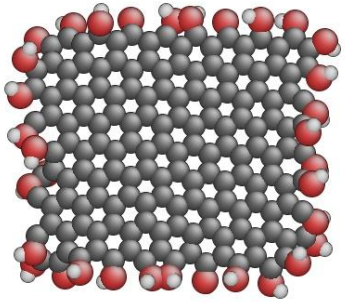
H-Terminated

542 C atoms

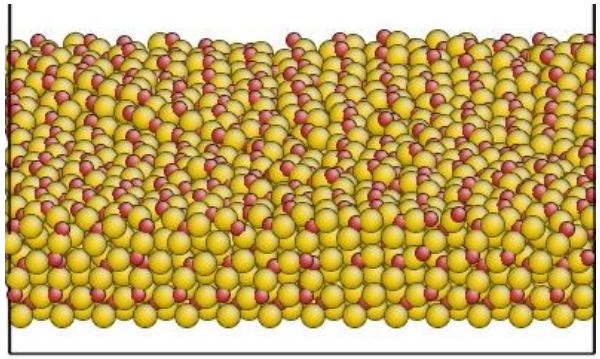


O Terminated

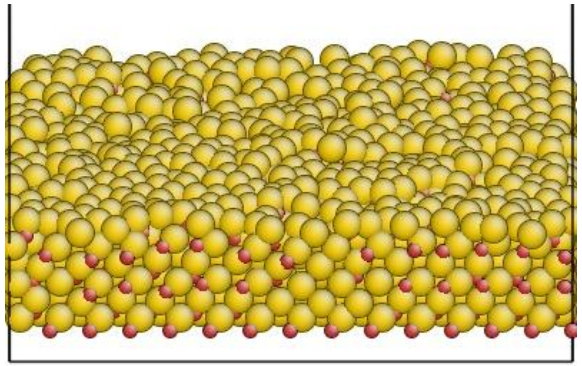
160 C atoms



OH Terminated

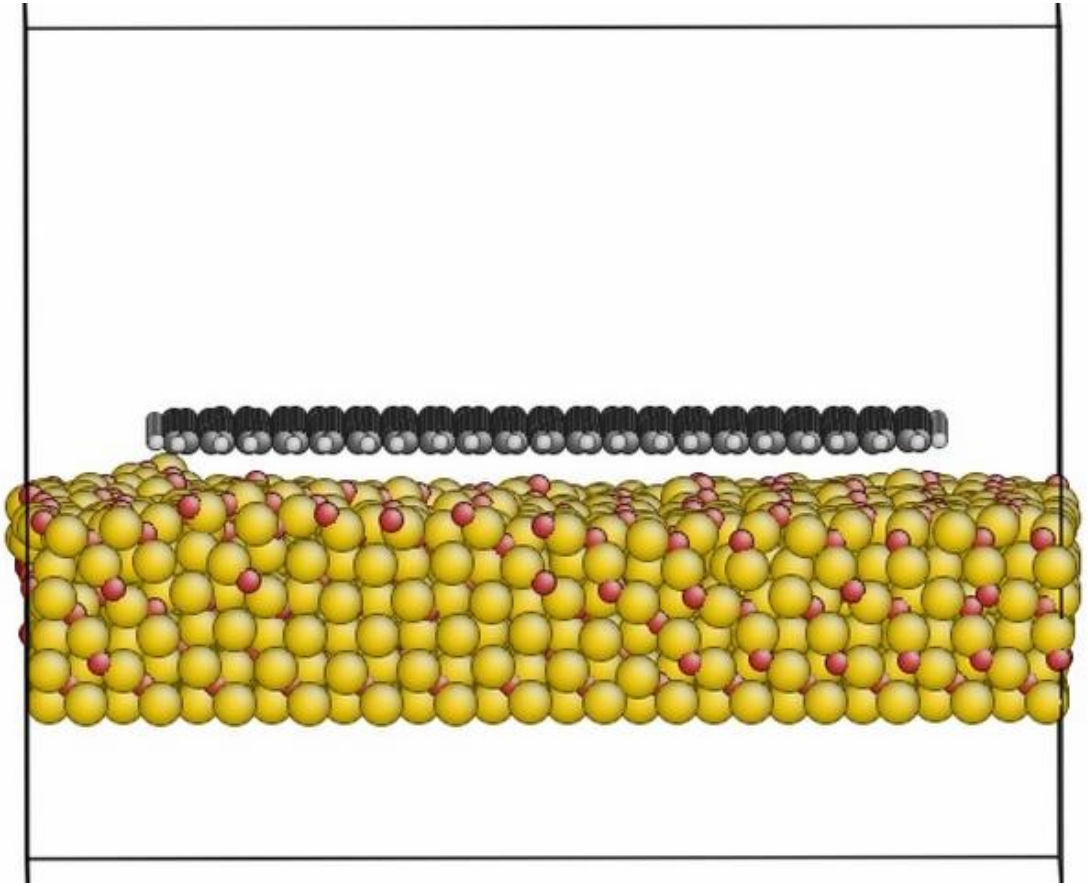


O-Termination

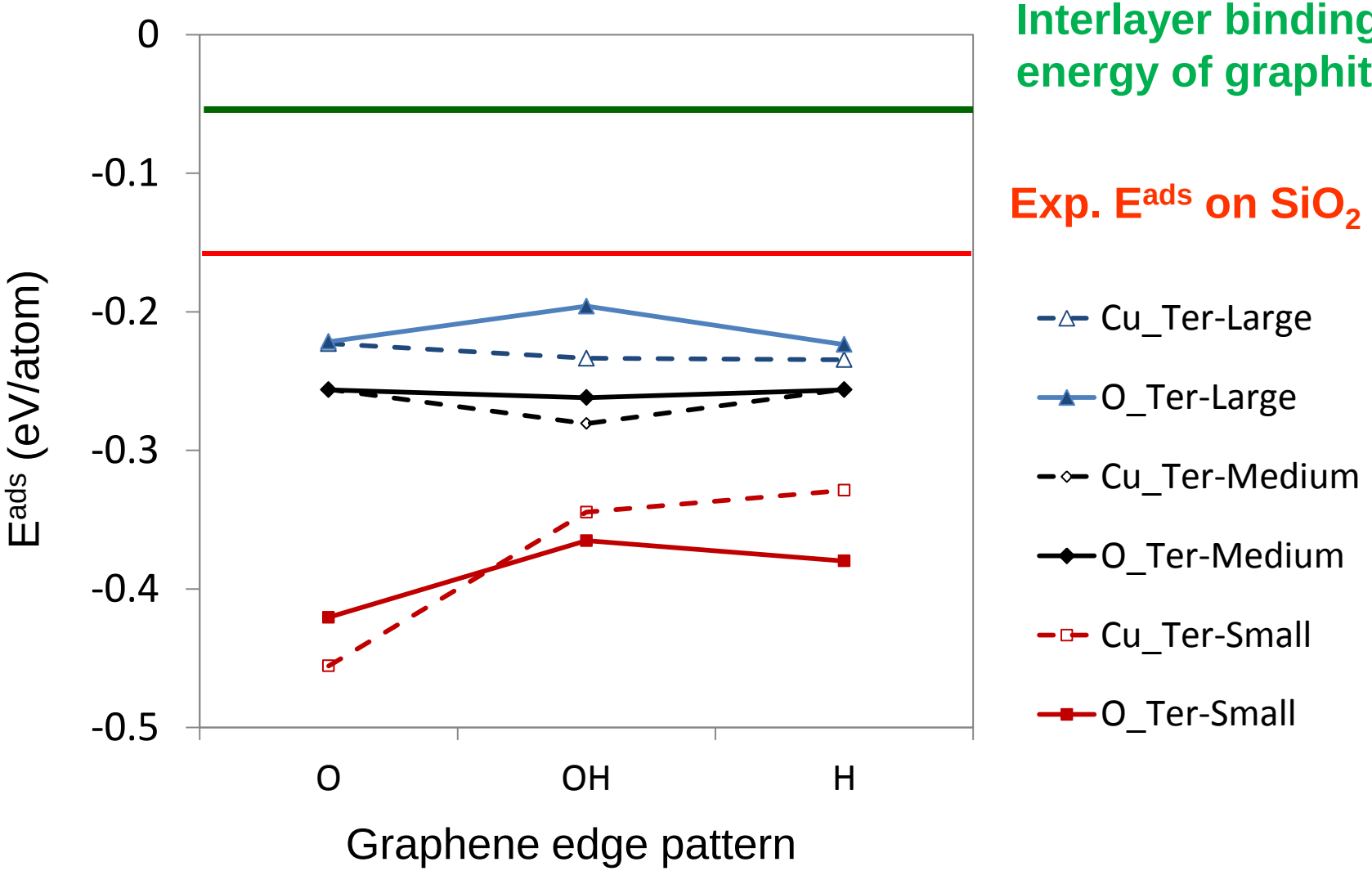


Cu-Termination

Graphene Adhesion on Cu_2O



Graphene Adhesion on Cu_2O



Koenig et al. Nature Nano, Sept., 2011.

Conclusions

- Have developed an empirical, variable charge many body (COMB) potential for modeling heterogeneous interfaces
- Successfully applied to atomic-scale simulations of systems consisting of discrete bonding types