

Reactive force fields: concepts of ReaxFF

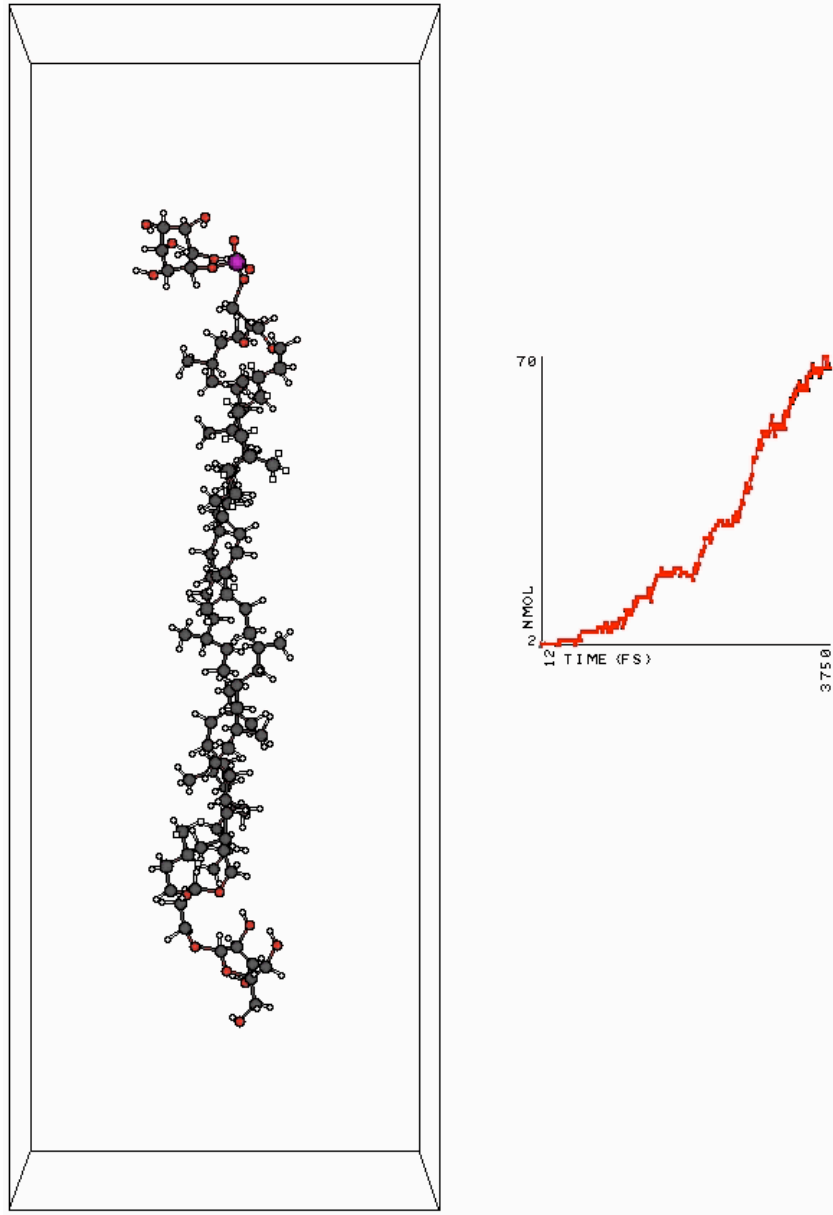
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CH-121 lecture February 4 2008



Aim: simulation of the dynamics of large, complicated reactive systems

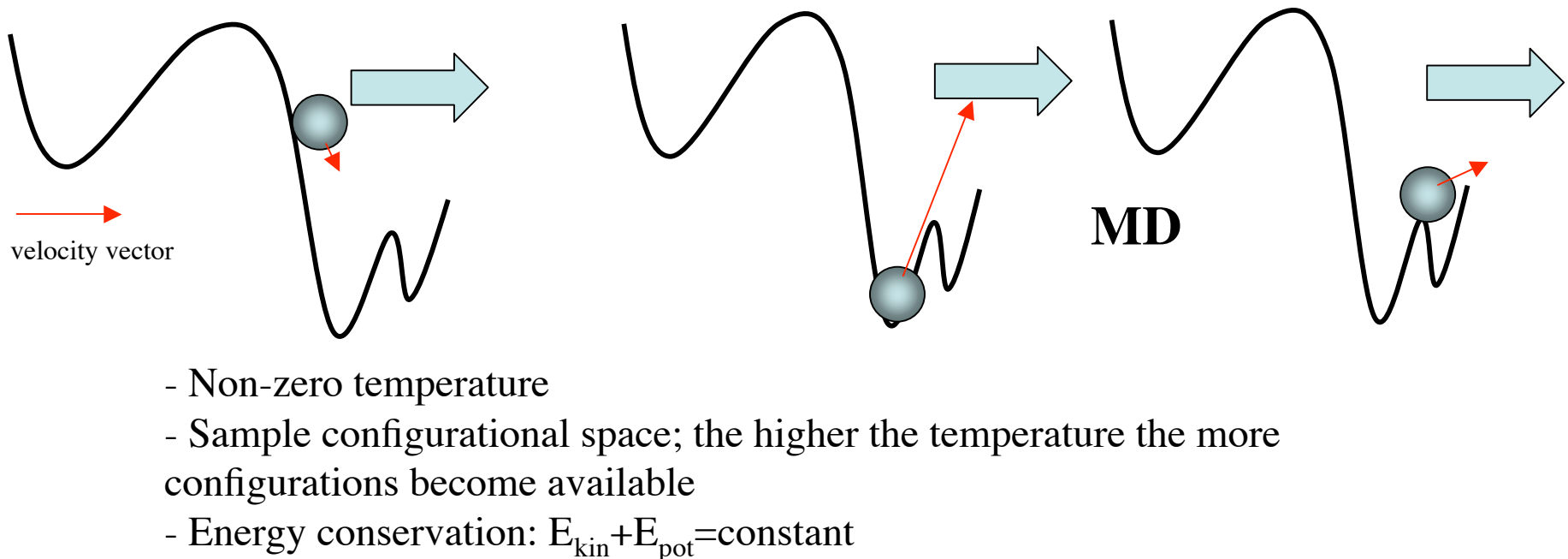
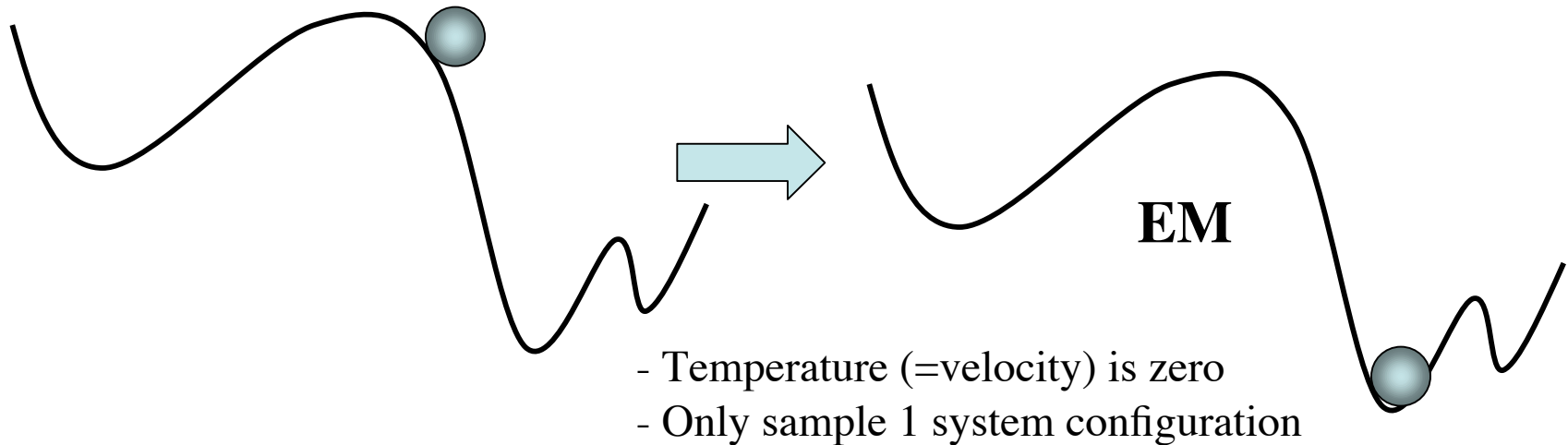


Simulation of the decomposition of a archaeol lipid biomarker by exposure to high-velocity (30eV) N-radicals

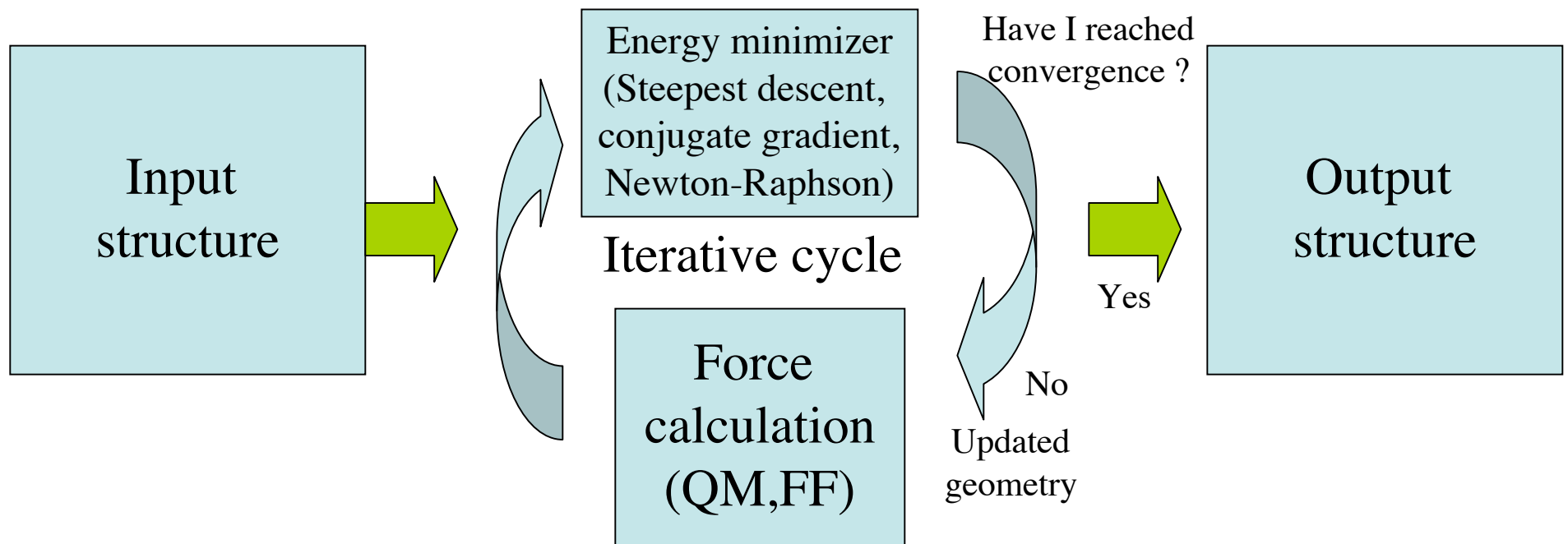
Outline

- Energy minimization and molecular dynamics methods
- Simulations on the dynamics of chemical reactions
- How to make a force field reactive: building the ReaxFF reactive force field
 - Concepts of covalent non-reactive force fields
 - Introduction of bond orders
 - Non-bonded interactions in a reactive force field
 - Charge polarization
 - Current status of the ReaxFF method
 - ReaxFF program, in- and output files
- Force field development for Si/SiO systems
- Applications of the Si/SiO reactive force field
 - Hydrogen diffusion in Si/SiO₂ interfaces
 - Thermal decomposition of PDMS polymers

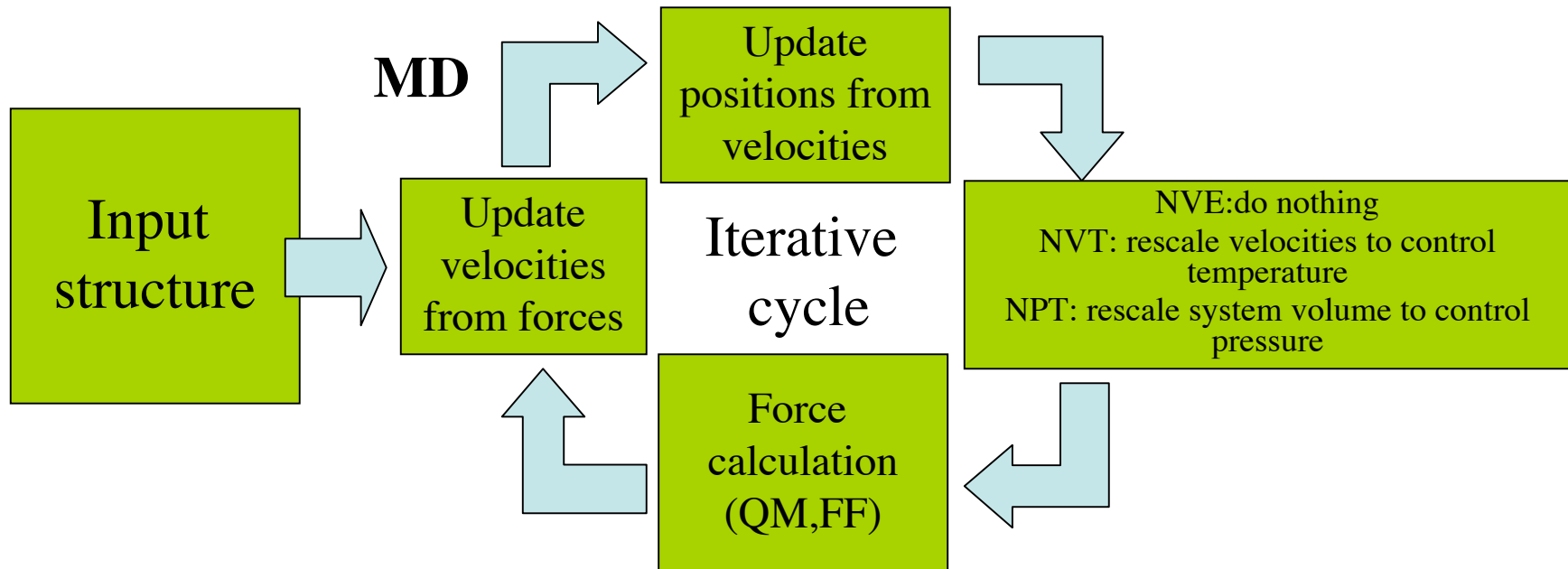
Energy minimization (EM) and molecular dynamics (MD) methods

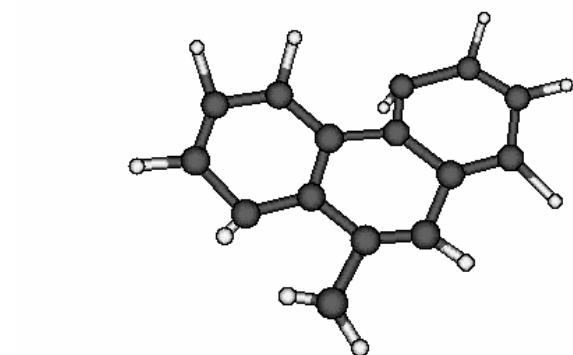


Energy minimization methods: structure



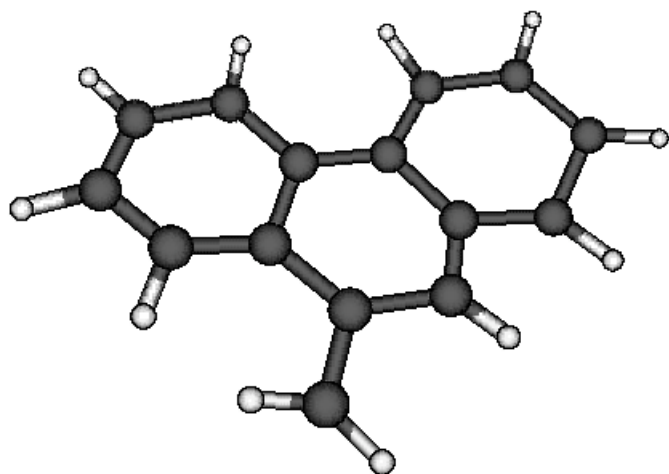
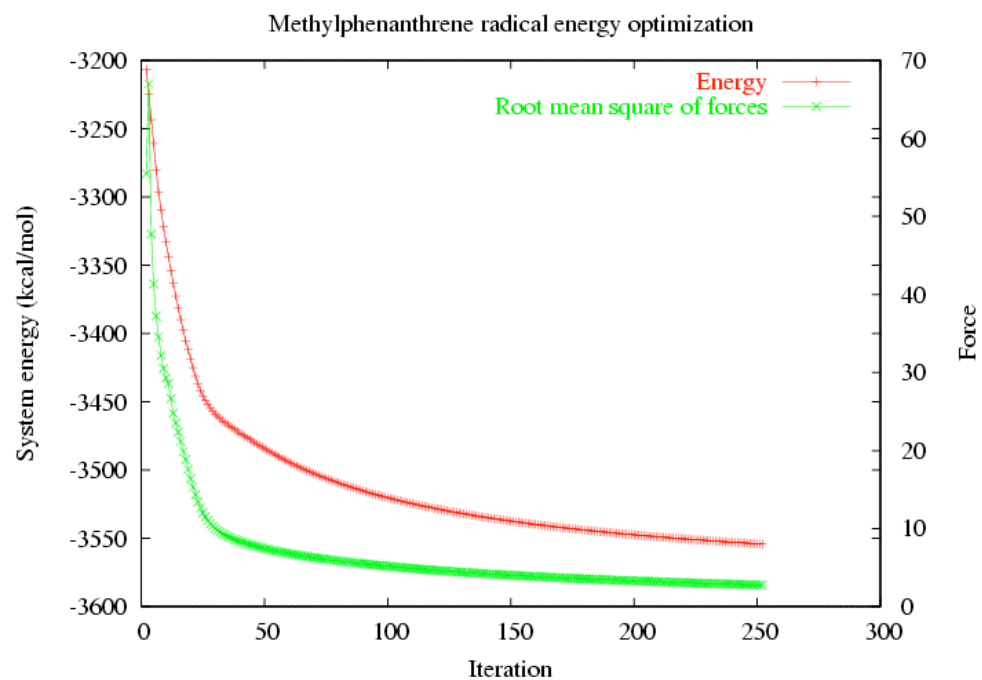
MD-methods: structure





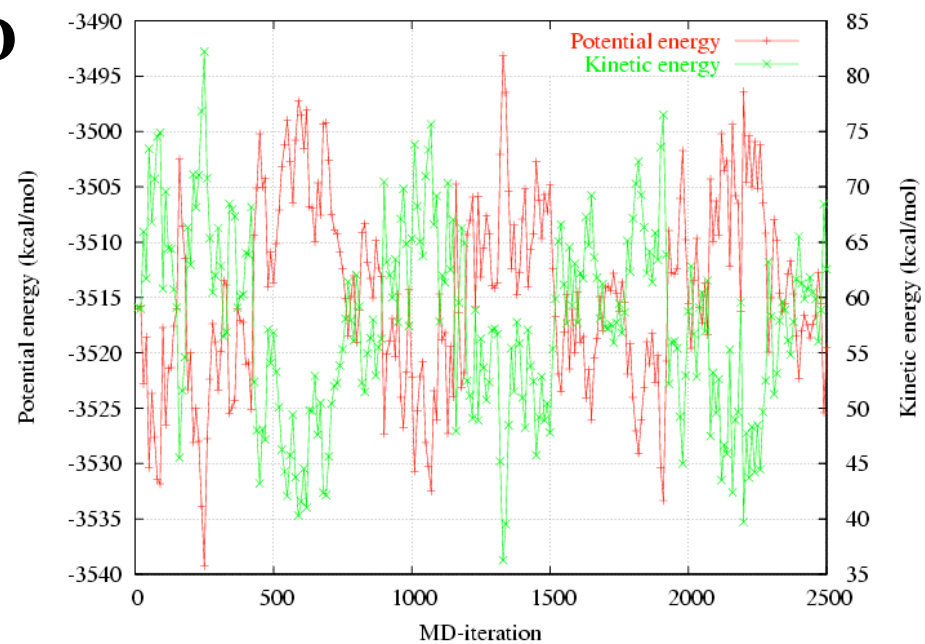
MM

FF energy minimization of a methylphenanthrene radical using a steepest descent method



MD

FF NVE molecular dynamics of a methylphenanthrene radical at T=700K



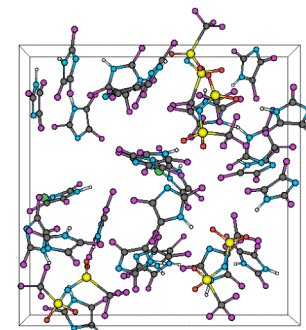
Applications of EM and MD

EM

- Determine static (0 Kelvin) properties of a single system configuration.
- Can be used to calculate IR, NMR-spectra, geometry information, relative energies.
- Usually employed on a single molecule; not relevant for multi-molecular systems.

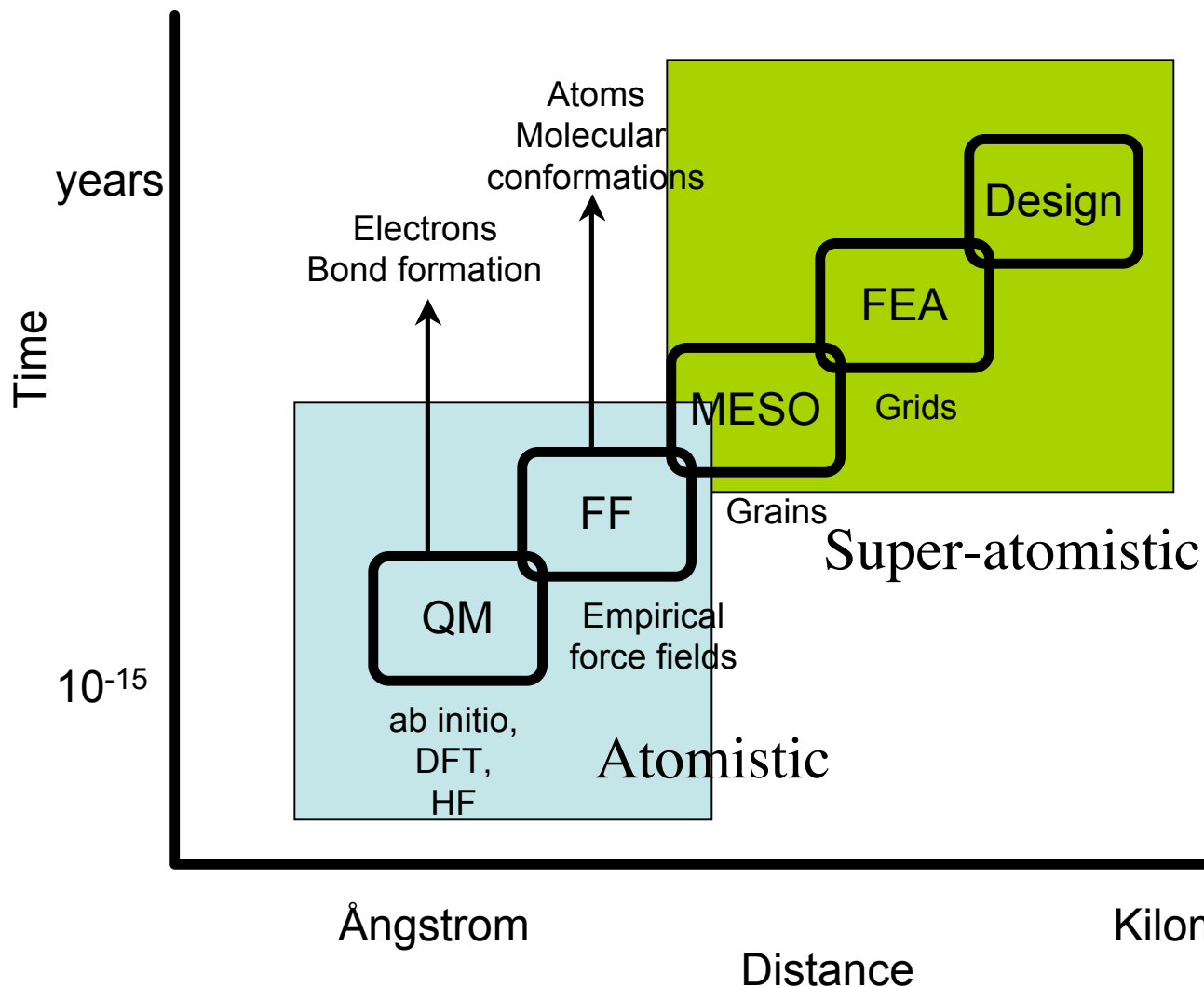
MD

- Used to sample the configurational space; average over multiple system configurations.
- Can be used to model temperature and pressure effects
- Can be used to calculate diffusion constants, reaction rates.
- Can be employed on multi-component systems.
- Almost always FF; QM/MD is very expensive



Fluorimidazole
/HTFS system

Simulations on the dynamics of chemical reactions



QM methods:

- Fundamental
- Expensive, only small systems

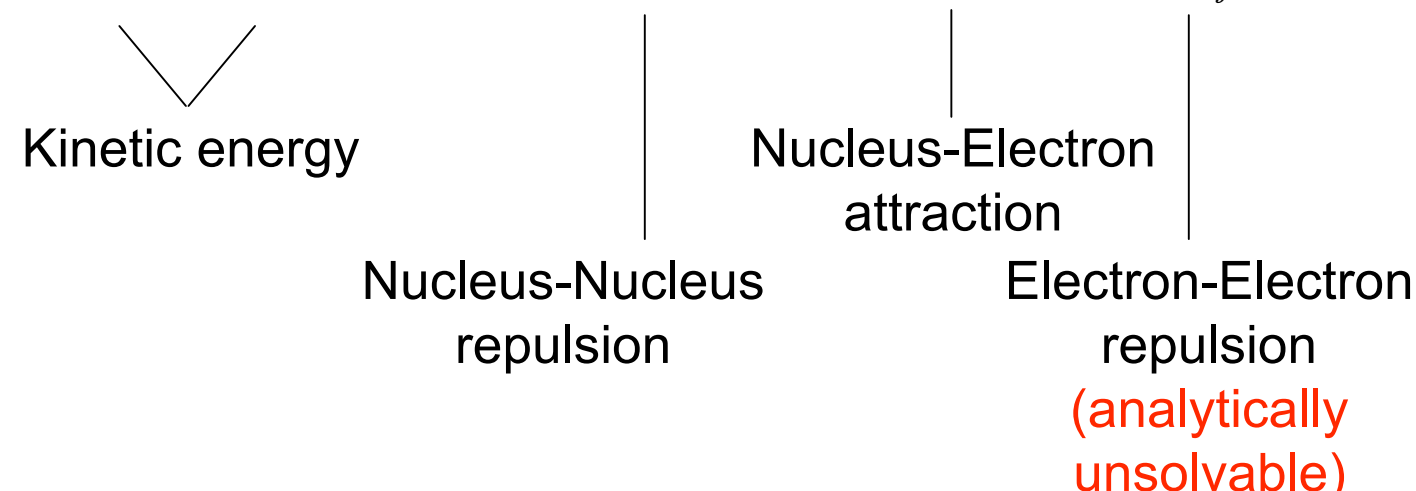
FF methods

- Empirical; need to be trained
- Much cheaper than QM, can be applied to much larger systems

QM-methods

$$\mathbf{H}\Psi = E\Psi$$

$$\mathbf{H} = - \sum_A \frac{1}{2M_A} \nabla_A^2 - \sum_i \frac{1}{2} \nabla_i^2 + \sum_{A < B} \frac{Z_A Z_B}{R_{AB}} - \sum_i \sum_A \frac{Z_A}{R_{Ai}} + \sum_{i < j} \frac{1}{r_{ij}}$$



Kinetic energy

Nucleus-Nucleus repulsion

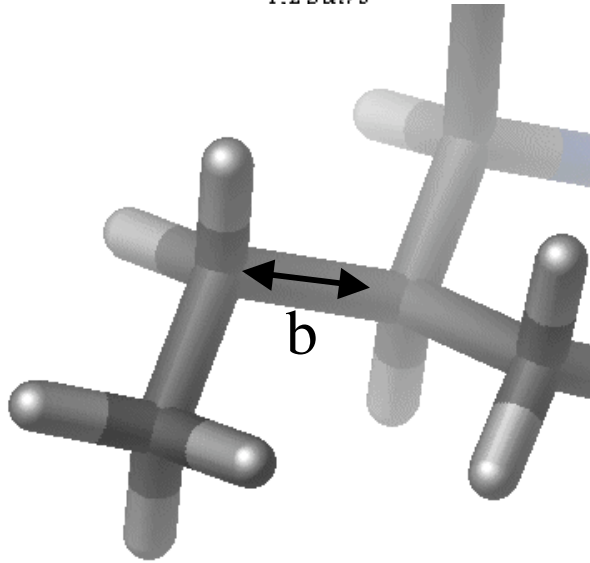
Nucleus-Electron attraction

Electron-Electron repulsion
(analytically unsolvable)

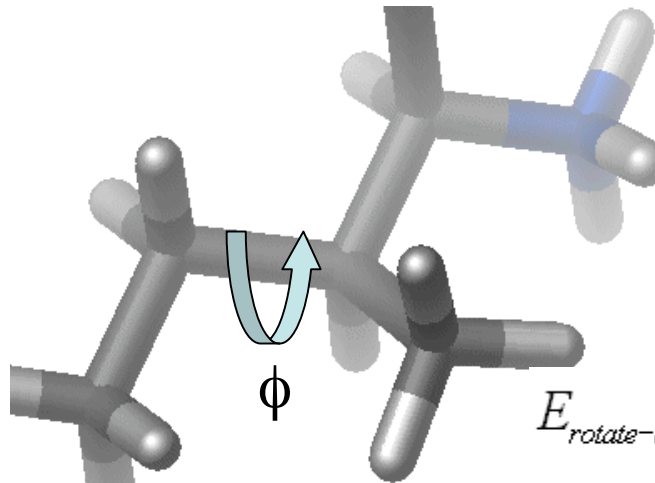
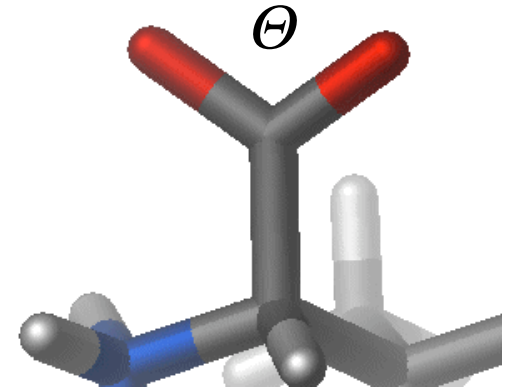
- Allows calculation of atomic interactions First Principles
- Computationally expensive, especially for finding accurate approximations of electron-electron repulsion term

Force field methods

$$E_{\text{bond-stretch}} = \sum_{1,2 \text{ pairs}} K_b (b - b_0)^2$$



$$E_{\text{bond-bend}} = \sum_{\text{angles}} K_\theta (\theta - \theta_0)^2$$

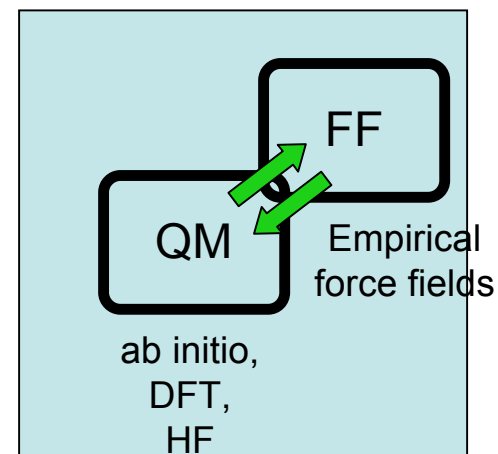


$$E_{\text{rotate-along-bond}} = \sum_{1,4 \text{ pairs}} K_\phi (1 - \cos(n\phi))$$

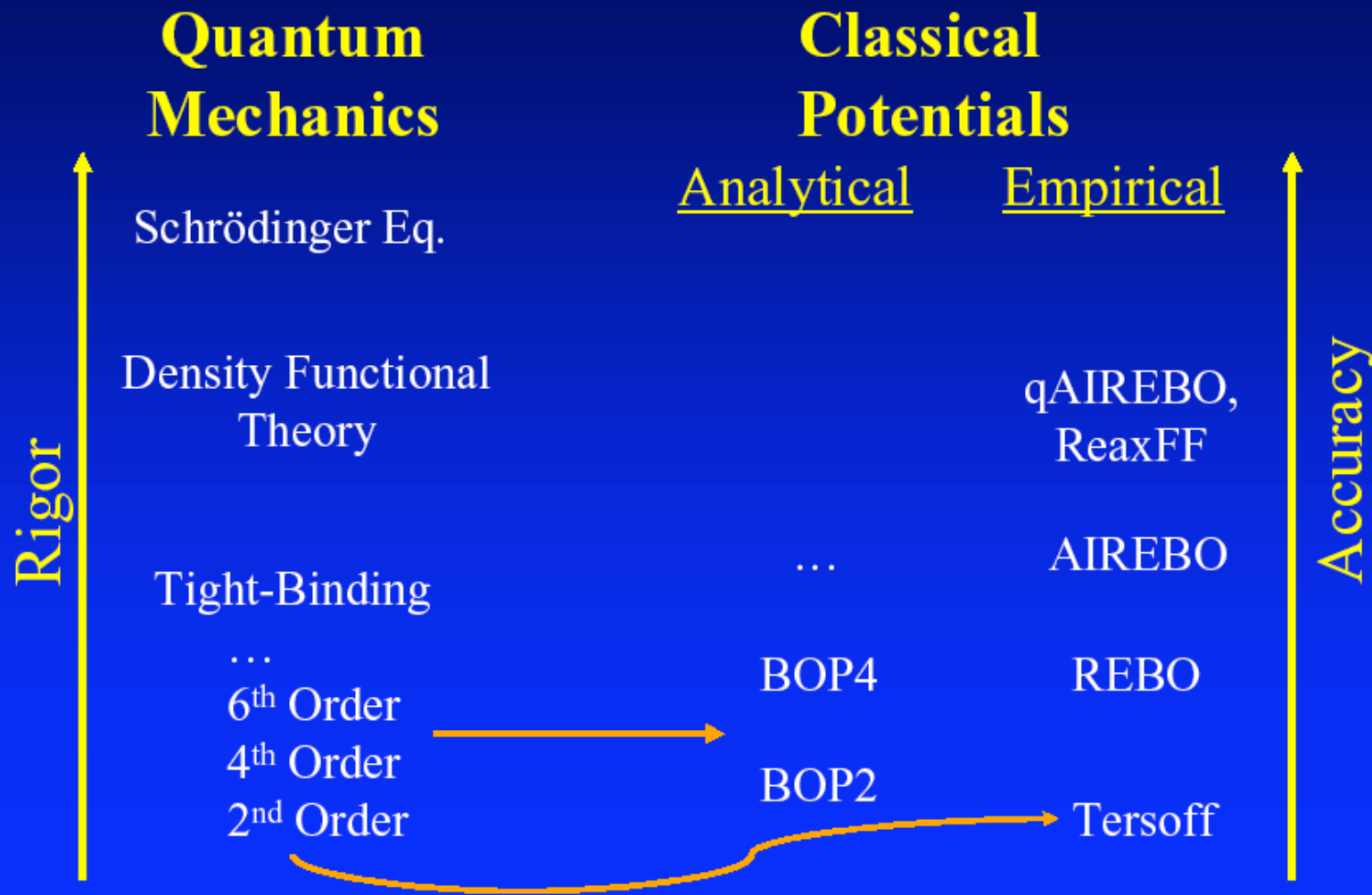
- Empirical, we need to derive values for the force field parameters (intuition, compare to experiment, compare to QM)
- MUCH faster than QM; can be applied to bigger systems

QM and FF-based approaches to reactive MD

- Option 1: Burn CPUs with QM/MD (e.g. Raty et al., PRL 2005)
- Option 2: use empirical assumptions to make QM faster (semi-empirical methods)
 - CINDO/MINDO/AM1/MOPAC (e.g. Pople and Segal, JCP 1966; Stewart, J. Comp. Chem. 1989)
 - Tight-binding (e.g. McMahan and Klepeis, PRB 1997)
 - Analytical Bond Order Potentials (e.g. Pettifor and Oleinik, PRB 1999)
- Option 3: Add ability to simulate reactions to FF-method (empirical bond-order based force fields)
 - Tersoff/Brenner /AIREBO (Tersoff, PRL 1988; Brenner, PRB 1990, Stuart et al., JCP 2000)
 - LCBOP (de Los et al., PRB 2005)
 - EDIP (e.g. Bazant and Kaxiras, PRL 1996)
 - ReaxFF (e.g. van Duin et al. JPC-A 2001)



Classes of Models



from Steve Stuart, Clemson University

How to make a force field reactive: building the ReaxFF reactive force field

- Concepts of covalent non-reactive force fields
- Introduction of bond orders
- Non-bonded interactions in a reactive force field
- Charge polarization
- Current status of the ReaxFF method
- ReaxFF program, in- and output files

Concepts of covalent non-reactive force fields

$$E_{system} = E_{bond} + E_{angle} + E_{torsion} + E_{vdWaals} + E_{Coulomb}$$

$$E_{bond} = k_b (r - r_o)^2$$

$$E_{angle} = k_v (\varphi - \varphi_o)^2$$

$$E_{torsion} = V_2 \cdot (1 - \cos 2\omega) + V_3 \cdot (1 + \cos 3\omega)$$

$$E_{vdWaals} = D_{ij} \left\{ \exp \left[\alpha_{ij} \cdot \left(1 - \frac{r_{ij}}{r_{vdW}} \right) \right] - 2 \cdot \exp \left[\frac{1}{2} \alpha_{ij} \cdot \left(1 - \frac{r_{ij}}{r_{vdW}} \right) \right] \right\}$$

$$E_{Coulomb} = C \cdot \frac{q_i \cdot q_j}{r_{ij}}$$

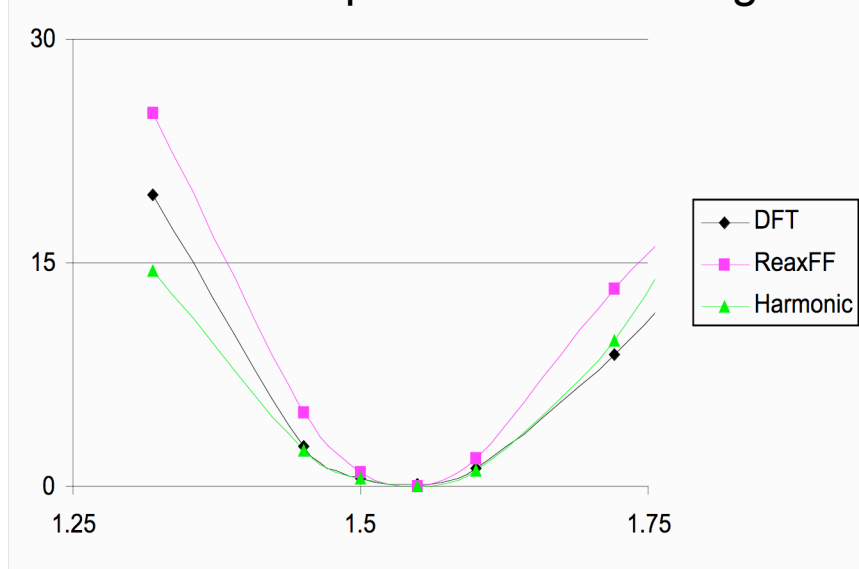
- Can be parameterized to describe structures and energies close to equilibrium
- Expansion with anharmonic terms improves reliability and application range
- Does not dissociate bonds properly

System energy description for a simple harmonic non-reactive force field

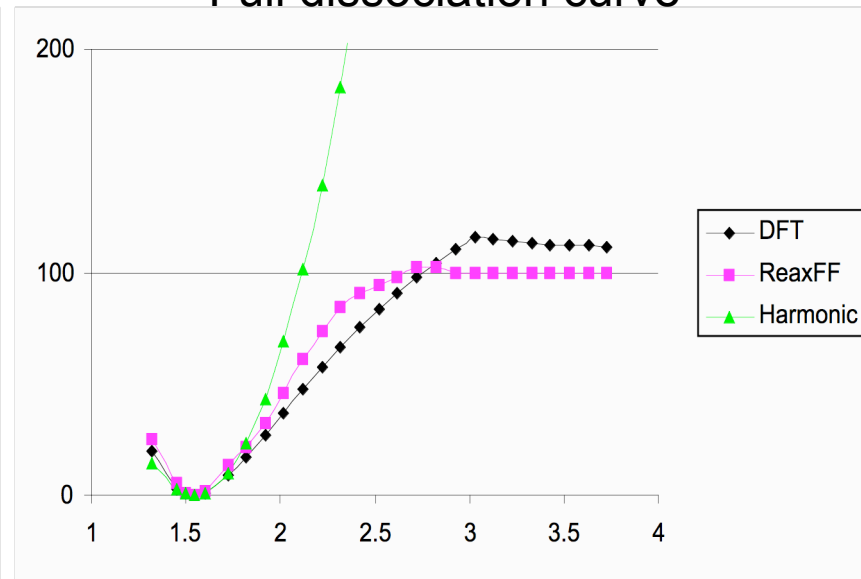
Failure of the harmonic model

C-C bond stretching in Ethane

Around the equilibrium bond length



Full dissociation curve



- Although the harmonic approximation can describe the bond stretching around the equilibrium it cannot describe the bond dissociation.
- Harmonic force field needs to use multiple atom types to distinguish single, double and triple bonded carbons.

From non-reactive to reactive force fields: key features of ReaxFF

-To get a smooth transition from nonbonded to single, double and triple bonded systems ReaxFF employs a bond length/bond order relationship. Bond orders are updated every iteration.

-All connectivity-dependent interactions (i.e. valence and torsion angles) are made bond-order dependent, ensuring that their energy contributions disappear upon bond dissociation.

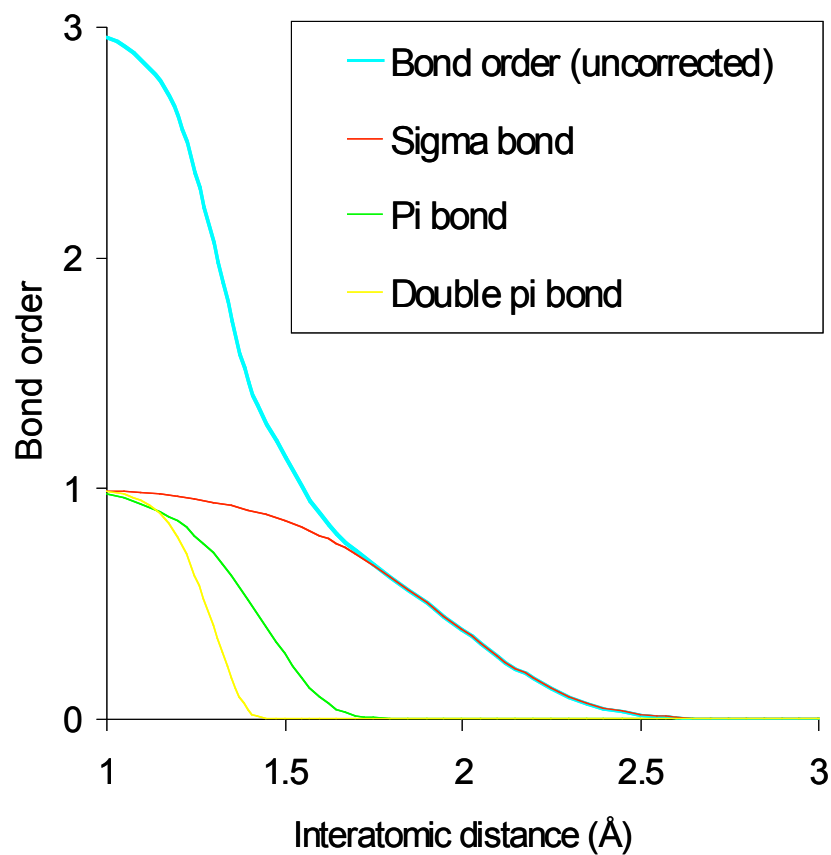
- Nonbonded interactions (van der Waals, Coulomb) are calculated between **every** atom pair, irrespective of connectivity. Excessive close-range nonbonded interactions are avoided by shielding.

- ReaxFF uses a geometry-dependent charge calculation scheme that accounts for polarization effects.

Introduction of bond orders

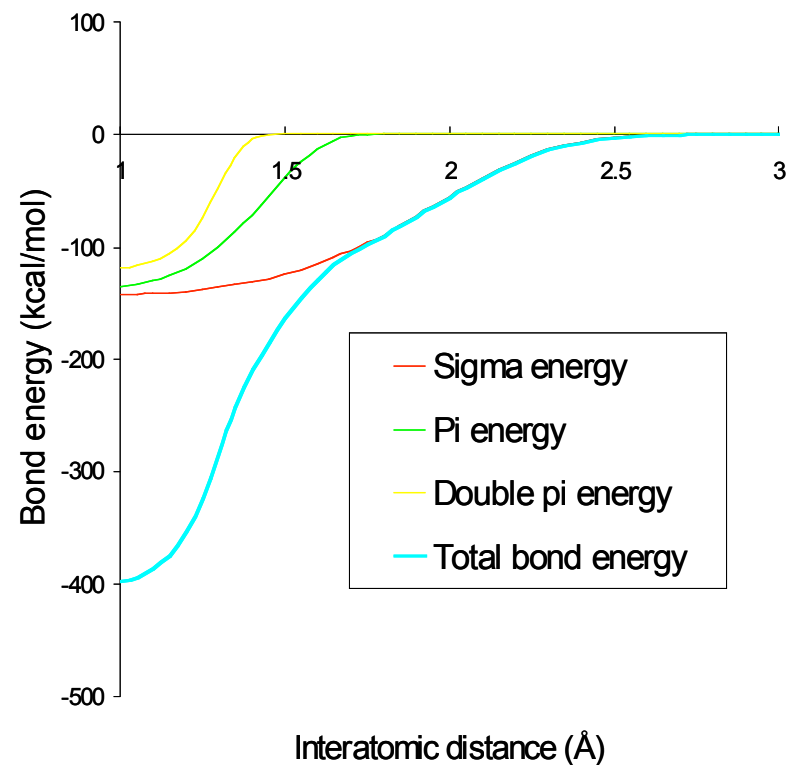
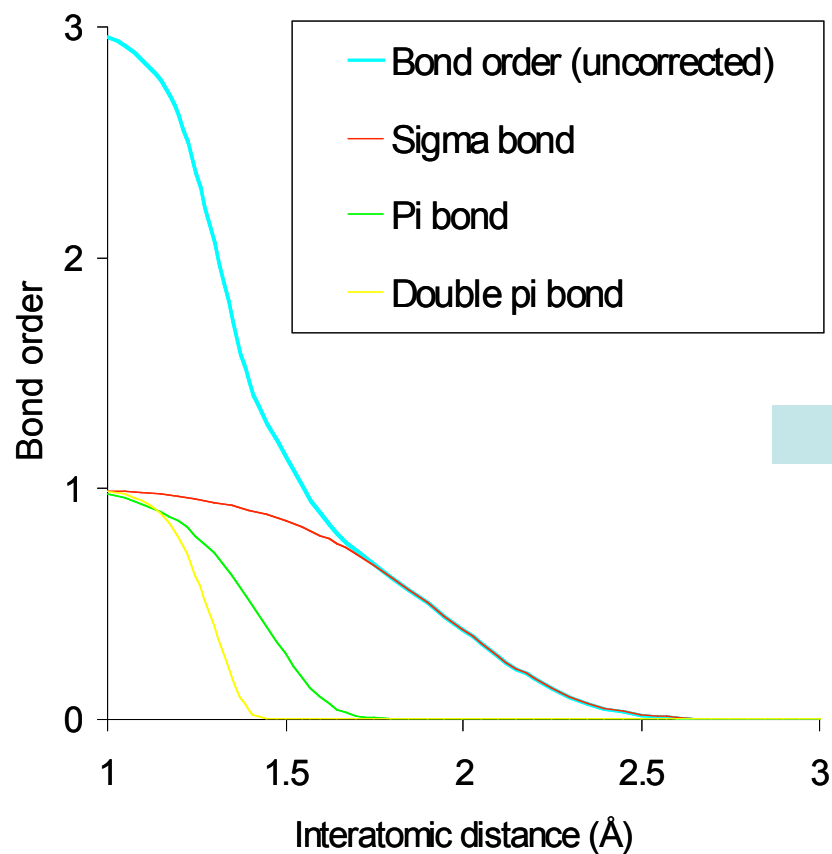
Calculation of bond orders from interatomic distances

$$BO_{ij}' = \exp \left[p_{bo,1} \cdot \left(\frac{r_{ij}}{r_o^\sigma} \right)^{p_{bo,2}} \right] + \exp \left[p_{bo,3} \cdot \left(\frac{r_{ij}}{r_o^\pi} \right)^{p_{bo,4}} \right] + \exp \left[p_{bo,5} \cdot \left(\frac{r_{ij}}{r_o^{\pi\pi}} \right)^{p_{bo,6}} \right]$$



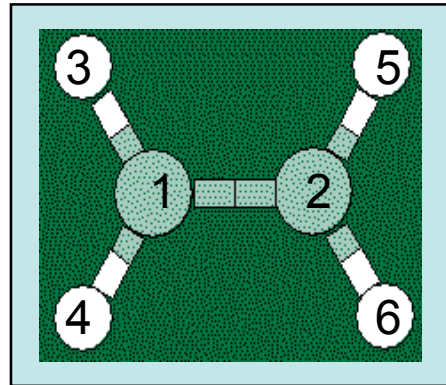
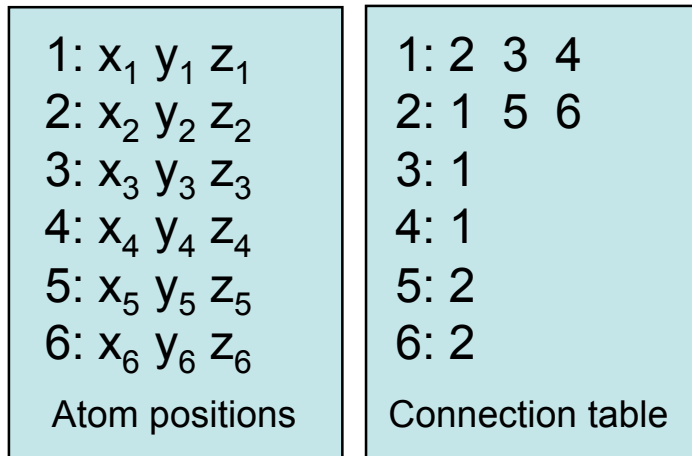
Calculation of bond energy from bond orders

$$E_{bond} = -D_e^\sigma \cdot BO_{ij}^\sigma \cdot f(BO_{ij}^\sigma) - D_e^\pi \cdot BO_{ij}^\pi - D_e^{\pi\pi} \cdot BO_{ij}^{\pi\pi}$$

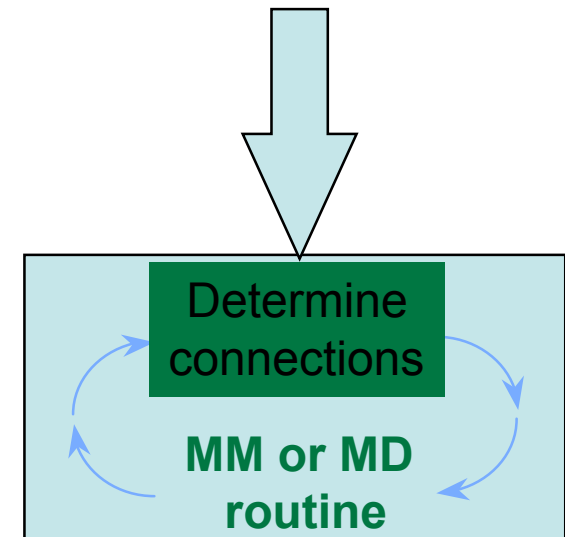
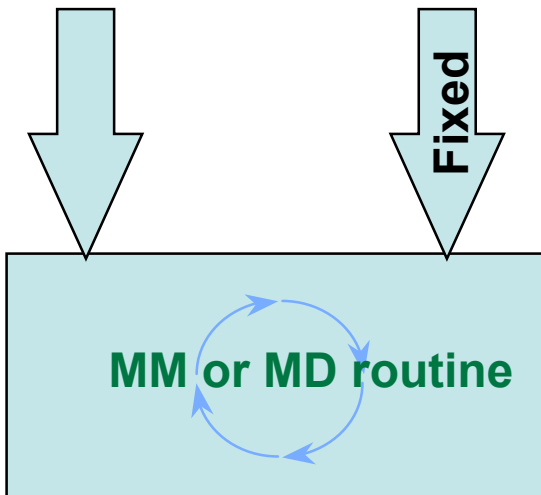
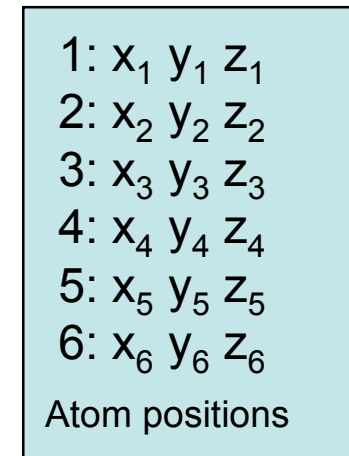


Connectivity: differences in program structure

Non-reactive force field

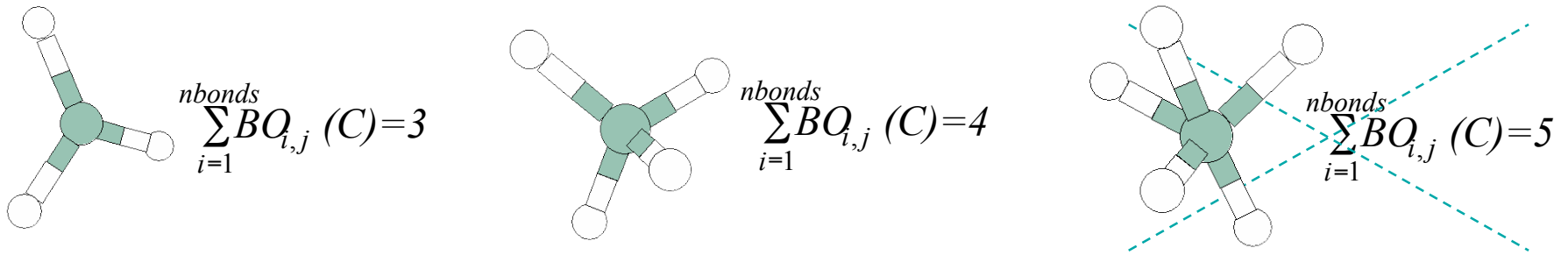


Reactive force field



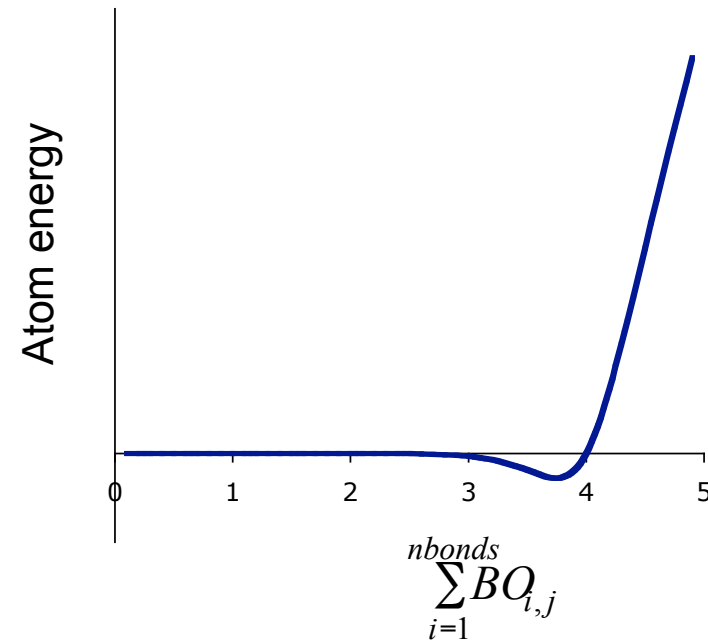
Dealing with overcoordination

Avoid unrealistically high amounts of bond orders on atoms



$$E_{over} = f(BO_{ij}) \cdot \Delta_i \cdot \frac{1}{1 + \exp(\lambda \cdot \Delta_i)}$$

$$\Delta_i = Valency_i - \sum_{j=1}^{neighbours} BO_{ij}$$



From non-reactive to reactive force fields: key features of ReaxFF

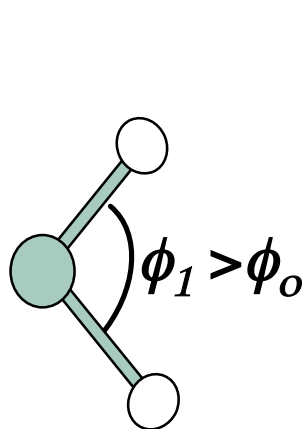
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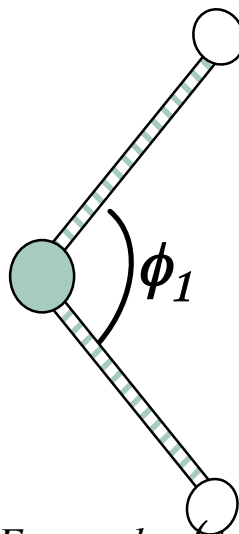
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-ReaxFF uses a geometry-dependent charge calculation scheme that accounts for polarization effects.

Valence angles

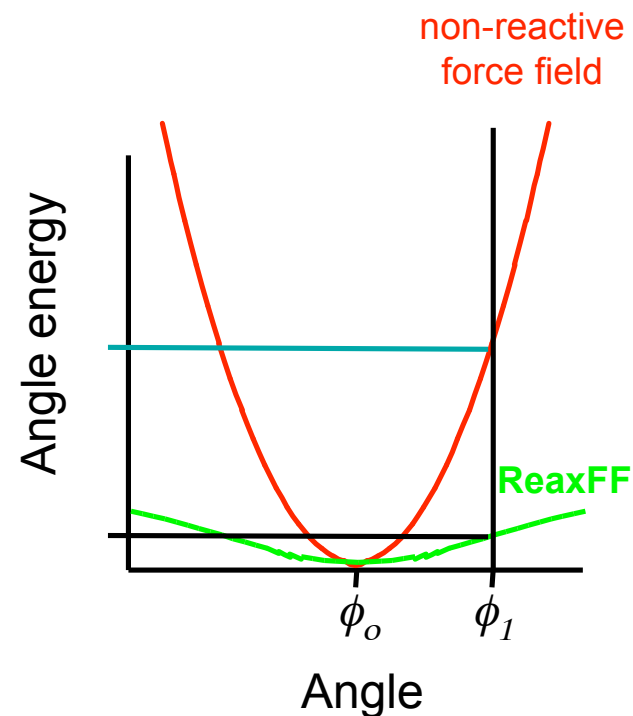


Bond orders: 1



$$E_{angle} = k_a \cdot (\phi - \phi_o)^2$$

Bond orders: 0.4



Non-reactive: $E_{angle} = k_a \cdot (\phi - \phi_o)^2$

Reactive: $E_{angle} = \underbrace{\left[1 - \exp(\lambda_3 \cdot BO_a^3)\right] \left[1 - \exp(\lambda_3 \cdot BO_b^3)\right]}_{\text{Bond-order dependent part}} \cdot \left\{ k_a - k_a \exp\left[-k_b \cdot (\phi - \phi_o)^2\right] \right\}$

Bond-order dependent part

BO_a = Bond order a
 BO_b = Bond order b
 ϕ = Angle
 ϕ_o = Equilibrium angle

Torsion and conjugation

- Torsion angle energy term

$$E_{tors} = f_{10}(BO_{ij}, BO_{jk}, BO_{kl}) \cdot \sin \Theta_{ijk} \cdot \sin \Theta_{jkl} \cdot \left[\frac{1}{2} V_1 \cdot (1 + \cos \omega_{ijkl}) + \frac{1}{2} V_2 \cdot \exp \left\{ p_{tor1} \cdot (2 - BO_{jk}^{\pi} - f_{11}(\Delta_j, \Delta_k))^2 \right\} \cdot (1 - \cos 2\omega_{ijkl}) + \frac{1}{2} V_3 \cdot (1 + \cos 3\omega_{ijkl}) \right]$$

- 4-body (torsion) conjugation term

$$E_{conj} = f_{12}(BO_{ij}, BO_{jk}, BO_{kl}) \cdot p_{cot1} \cdot \left[1 + (\cos^2 \omega_{ijkl} - 1) \cdot \sin \Theta_{ijk} \cdot \sin \Theta_{jkl} \right]$$

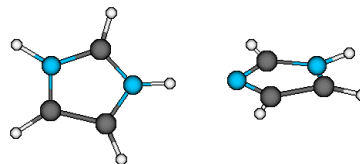
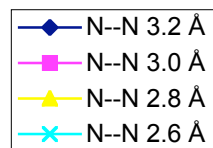
- Bond order dependent
- Tested against a large database of PAH heats of formation

- 3-body (angle) conjugation term

$$E_{coa} = p_{coa1} \cdot \frac{1}{1 + \exp(p_{coa2} \cdot \Delta_j^{val})} \cdot \exp \left[-p_{coa3} \cdot \left(-BO_{ij} + \sum_{n=1}^{neighbours(i)} BO_{in} \right)^2 \right] \cdot \exp \left[-p_{coa3} \cdot \left(-BO_{jk} + \sum_{n=1}^{neighbours(i)} BO_{kn} \right)^2 \right] \cdot \exp \left[-p_{coa4} \cdot (BO_{ij} - 1.5)^2 \right] \cdot \exp \left[-p_{coa4} \cdot (BO_{jk} - 1.5)^2 \right]$$

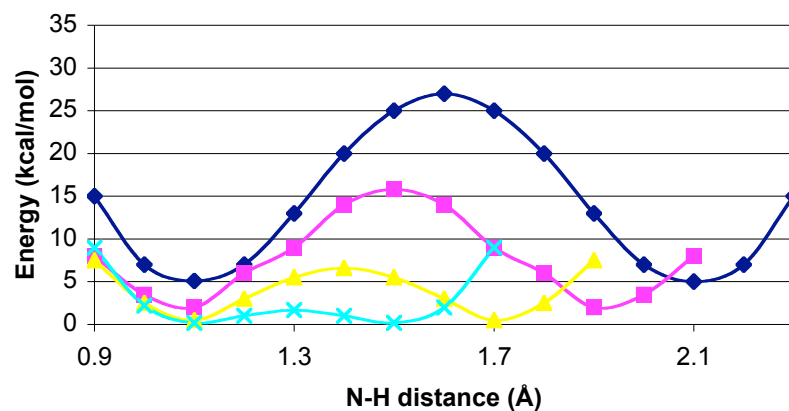
Hydrogen bonds

$$E_{Hbond} = p_{hb1} \cdot [1 - \exp(p_{hb2} \cdot BO_{XH})] \cdot \exp\left[p_{hb3} \left(\frac{r_{hb}^o}{r_{HZ}} + \frac{r_{HZ}}{r_{hb}^o} - 2\right)\right] \cdot \sin^8\left(\frac{\Theta_{XHZ}}{2}\right)$$

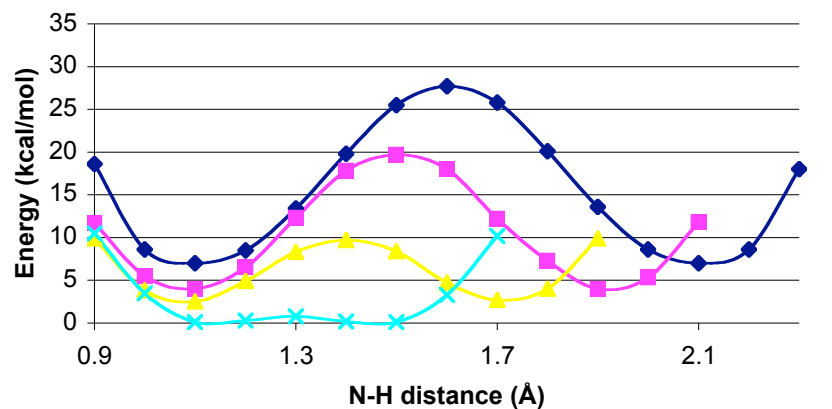


- Bond order dependent
- Tested for a wide range of hydrogen transfer reactions
- Tested for bulk water and proton diffusion in water

H-transfer in [Im-Im]⁺: QM-data



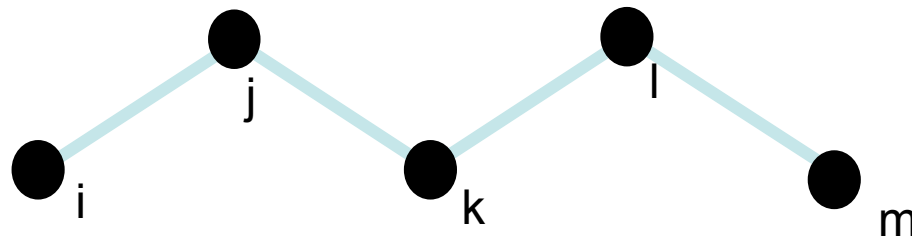
H-transfer in [Im-Im]⁺: ReaxFF-data



Key features

- To get a smooth transition from nonbonded to single, double and triple bonded systems ReaxFF employs a bond length/bond order relationship. Bond orders are updated every iteration.
- All connectivity-dependent interactions (i.e. valence and torsion angles) are made bond-order dependent, ensuring that their energy contributions disappear upon bond dissociation.
- Nonbonded interactions (van der Waals, Coulomb) are calculated between **every** atom pair, irrespective of connectivity. Excessive close-range nonbonded interactions are avoided by shielding.
- ReaxFF uses a geometry-dependent charge calculation scheme that accounts for polarization effects.

Nonbonded interactions



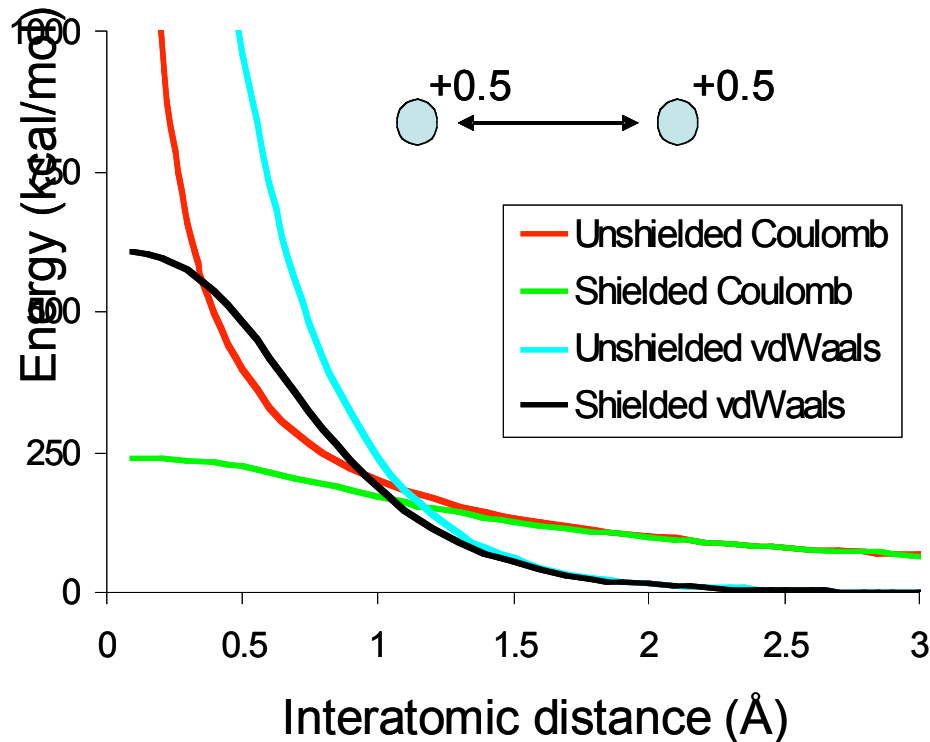
Non-reactive force field: ignore vdWaals and Coulomb interactions between atoms sharing a bond (i-j, j-k, k-l and l-m) or a valence angle (i-k, j-l and k-m).

These exception rules are very awkward when trying to describe reactions.

ReaxFF: calculate nonbonded interactions between *all* atom pairs, regardless of connectivity.

To avoid excessive repulsive/attractive nonbonded interactions at short distances both Coulomb and van der Waals interactions are shielded in ReaxFF.

Shielded vdWaaals and Coulomb interactions



$$E_{Coulomb} = C \cdot \frac{q_i \cdot q_j}{\left\{ r_{ij}^3 + \left(1 / \gamma_{ij} \right)^3 \right\}^{1/3}}$$

Shielded Coulomb
potential

vdWaaals: Shielded Morse potential

- For metals ReaxFF only uses bond energy, overcoordination, vdWaaals and Coulomb-terms (no angle or dihedrals)
- vdWaaals and overcoordination terms serve as a density-dependent repulsive term (as used in EAM-potentials [Daw and Baskes, PRB 1984]), allowing ReaxFF to describe bulk metals

Key features

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Charge polarization

- Assign one electronegativity and hardness to each element; optimize these parameters against QM-charge distributions
- Use system geometry in solving electronegativity equilibration equations in every iteration

$$\frac{\partial E}{\partial q_1} = \chi_1 + 2q_1\eta_1 + C \cdot \sum_{j=1}^n \frac{q_j}{\left(r_{1,j}^3 + \left(\frac{1}{\gamma_{1,j}} \right)^3 \right)^{\frac{1}{3}}}$$

$$\frac{\partial E}{\partial q_2} = \chi_2 + 2q_2\eta_2 + C \cdot \sum_{j=1}^n \frac{q_j}{\left(r_{2,j}^3 + \left(\frac{1}{\gamma_{2,j}} \right)^3 \right)^{\frac{1}{3}}}$$

.....

.....

$$\frac{\partial E}{\partial q_n} = \chi_n + 2q_n\eta_n + C \cdot \sum_{j=1}^n \frac{q_j}{\left(r_{n,j}^3 + \left(\frac{1}{\gamma_{n,j}} \right)^3 \right)^{\frac{1}{3}}}$$

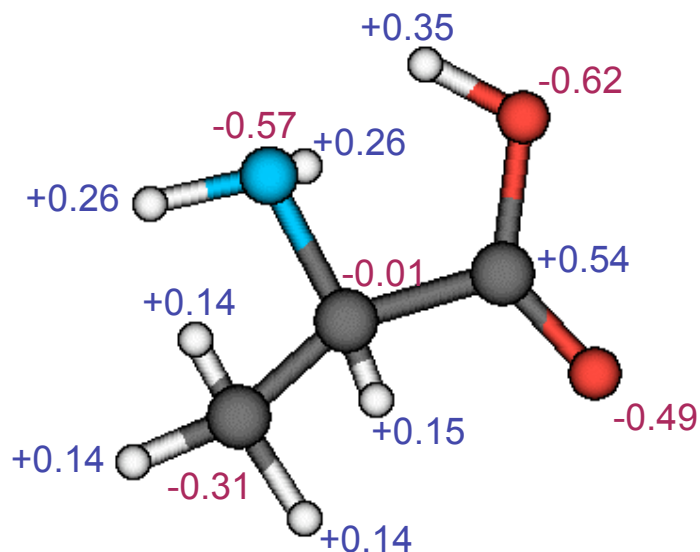
$$\sum_{i=1}^n q_i = 0$$

EEM-method
(Mortier et al., JACS
1986); shielding:
Janssens et al.
J.Phys.Chem. 1995.

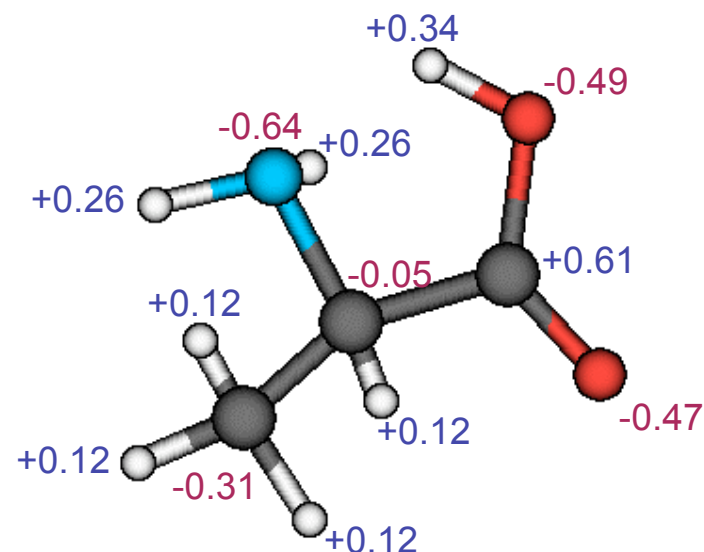
Similar to Qeq-method
(Rappe and Goddard, J.
Phys. Chem. 1991) with
empirical shielding
correction.

χ : atom electronegativity
 η : atom hardness
 γ : shielding parameter
 r : interatomic distances
 q : atom charge

ReaxFF charges



QM
Mulliken charges
DFT; 6-31G**

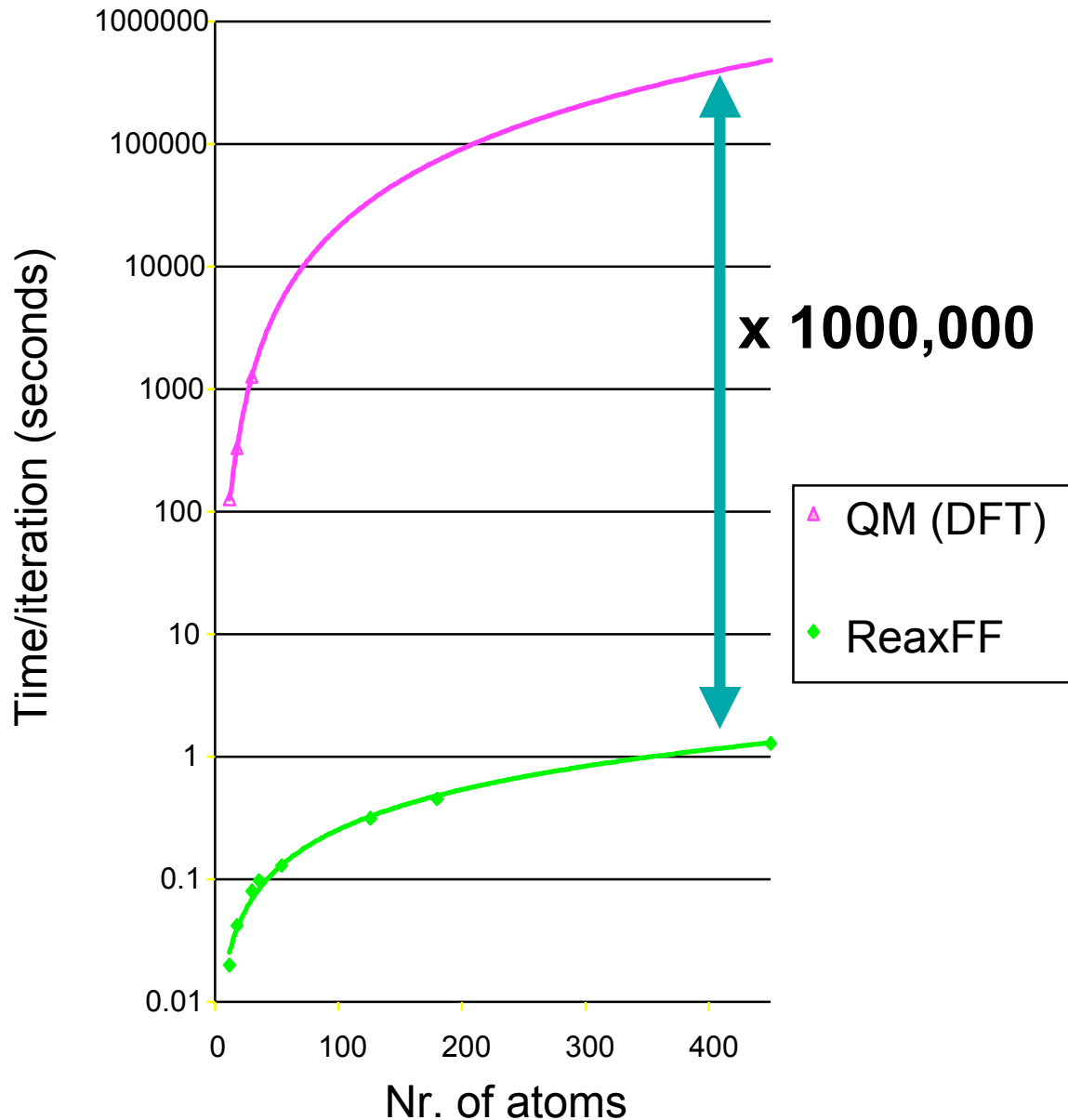


- Good reproduction of Mulliken charges (similar concepts)
- Combined with 1-2 Coulomb-interactions, this enables ReaxFF to simulate polarization effects on local chemistry
- EEM/Qeq methods work well around equilibrium; incorrect description of charge flow at high compression and dissociation (Chen and Martinez, Chem.Phys.Lett. 2006)
- Most expensive part of the reactive force field; needs to be updated every MD-step and forces sub-femtosecond steps

General rules for ReaxFF

- MD-force field; no discontinuities in energy or forces even during reactions.
- User should not have to pre-define reactive sites or reaction pathways; potential functions should be able to automatically handle coordination changes associated with reactions.
- Each element is represented by only 1 atom type in the force field; force field should be able to determine equilibrium bond lengths, valence angles etc. from chemical environment.

ReaxFF Computational expense



- ReaxFF allows for reactive MD-simulations on systems containing more than 1000 atoms
- ReaxFF is 10-50 times slower than non-reactive force fields
- Better scaling than QM-methods ($N\log N$ for ReaxFF, N^3 (at best) for QM)

Current development status of ReaxFF

- ReaxFF combines covalent, metallic and ionic elements allowing applications all across the periodic table
- All ReaxFF descriptions use the same potential functions, enabling application to interfaces between different material types
- Code has been distributed to over 60 research groups
- Parallel ReaxFF (GRASP/Reax and USC/Reax) available

ReaxFF transferability

Legend:

- alkali metals
- alkaline earth metals
- transition metals
- other metals
- other nonmetals
- halogens
- noble gases
- lanthanides
- actinides

not currently described by ReaxFF

Some ReaxFF publications

- C/H: van Duin et al, JPC-A 2001, 105, 9396; Org. Geochem. 2003, 34, 515; Chen et al, PR-B 2005, 72, 085416, Han et al. Appl. Phys. Lett. 2005, 86, 203108.
- C/N/O/H: Strachan et al, PRL 2003, 91, 09301; JCP 2005, 122, 054502; van Duin et al, JACS 2005, 127, 11053
- Metals: Zhang et al, PRB 2004, 69, 045423; Nielson et al., JPC-A 2005, 109, 493; Su et al., PRB 75, 2007; Ludwig et al, JPC-B 2006; Cheung et al, JPC-A 2005, 109, 851
- Si/SiO/SiC: van Duin et al., JPC-A 2003, 107, 3803; Chenoweth et al., JACS 2005, 127, 7192; Buehler et al., PRL 2006, 96, 095505; Buehler et al, PRL 2007.

Parallel ReaxFF: GRASP/ReaxFF

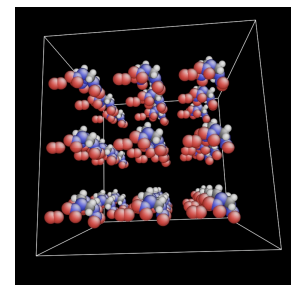
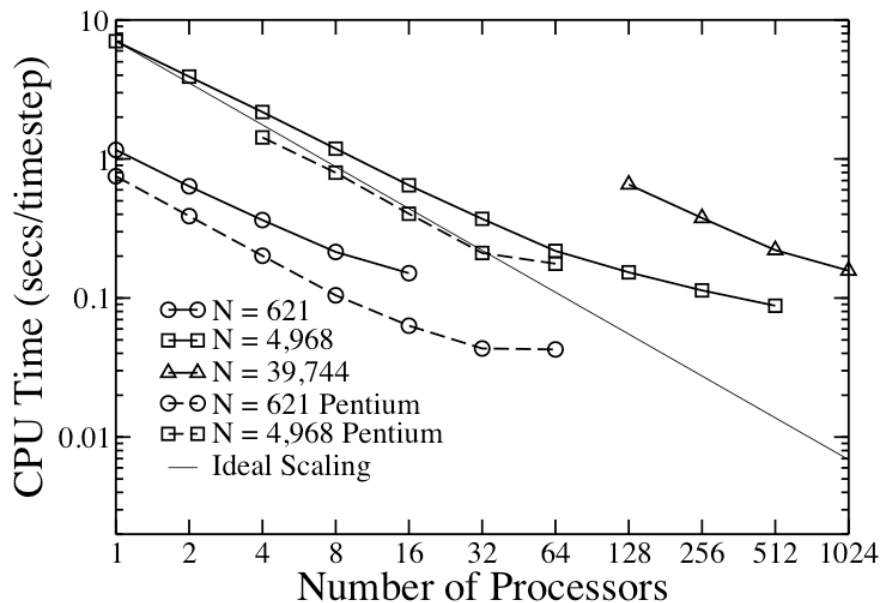
- ReaxFF is incorporated in the Grasp-framework (Aidan Thompson, Sandia) allowing parallel ReaxFF-simulations.

GRASP Performance on BG/L with ReaxFF

Comparison with Liberty Cluster (3GHz Pentium+Myrinet)

RDX Explosive with Oxygen

ReaxFF force field with charge equilibration



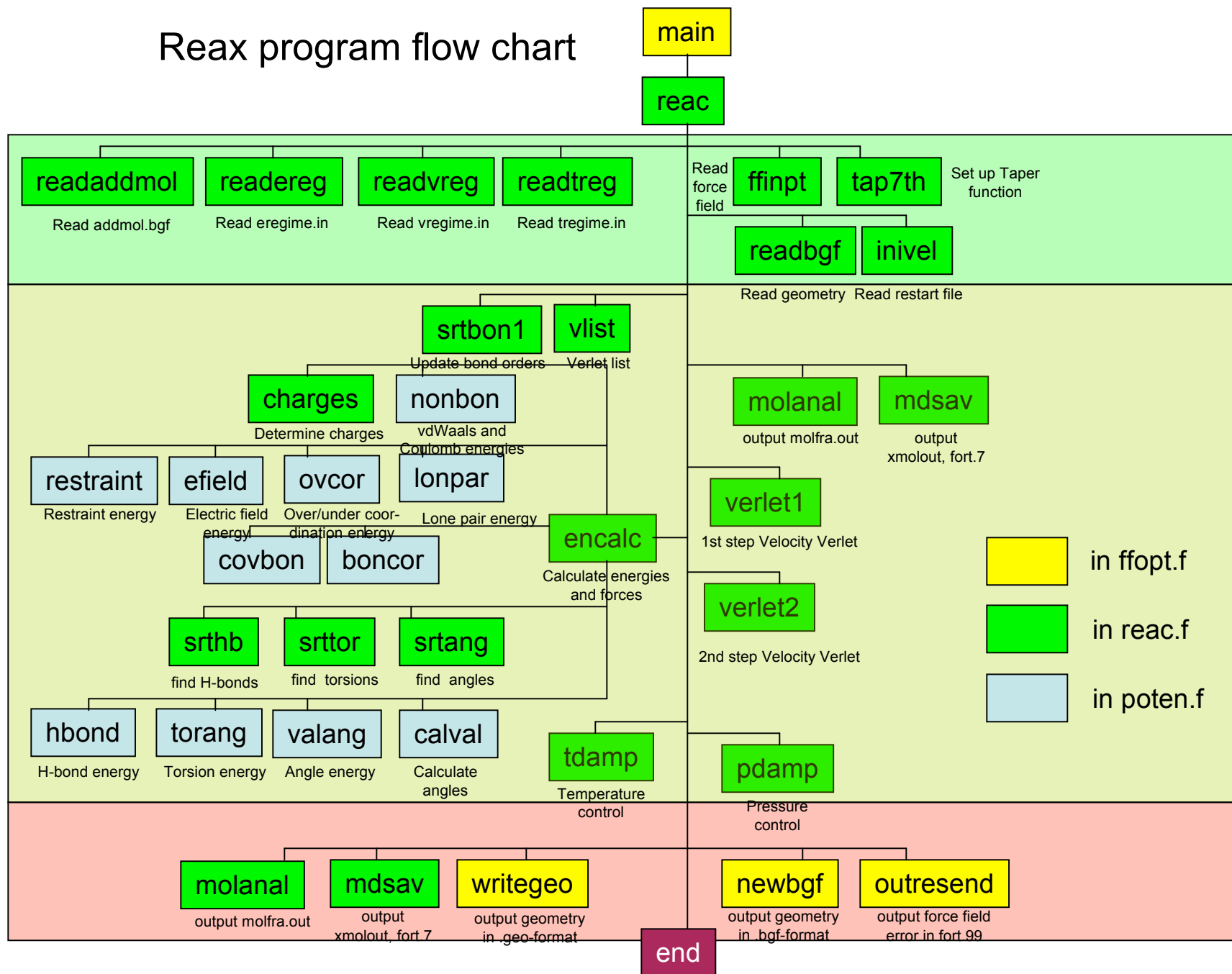
- ReaxFF enables reactive modelling
- Si/SiO₂, Explosives, film growth
- Each process computes energy and forces for a virtual non-periodic cluster
- Low communication, duplicated computation $\sim P(N/P)^{2/3}$
- Uses Van Duin's Fortran subroutines for force calculation.
- Good strong scaling
- Sweet spot: 5000 atoms/processor

ReaxFF program, in- and output files

ReaxFF program structure

- Written in Fortran-77
- Library independent
- Text-based interface (graphical interface is developed within CMDf)
- Installed on various computers and operating systems (Linux, Windows, Macs)
- Code divided in 6 parts:
 - reac.f (10640 lines): general MD routines
 - poten.f (3034 lines): energy equations
 - ffopt.f (1581 lines): force field optimization
 - shanno (1718 lines): energy minimization
 - vibra.f (1194 lines): vibrational frequencies
 - blas.f (613 lines): BLAS-routines
 - program parameters in cbka.blk

Reax program flow chart



Overview ReaxFF in- and output files

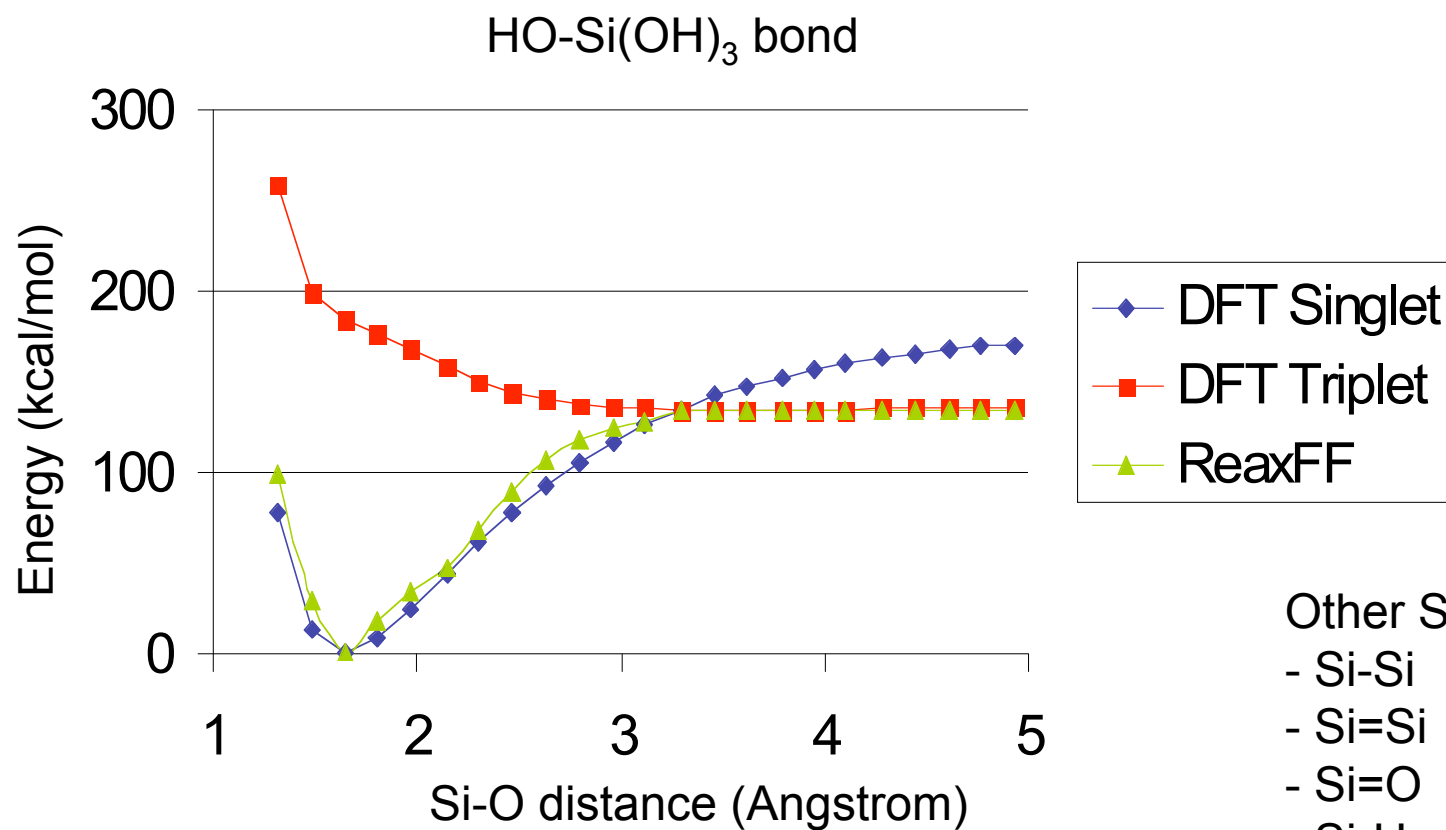
Mandatory input files

- geo (input geometry)
- control (run control parameters)
- ffield (force field parameters)
- exe (UNIX-script)

Force field development for Si/SiO systems

- Concept: build a QM-based database (training set) that described reactive and non-reactive aspects of the material and optimize ReaxFF to reproduce these QM-data.
- Bigger (more extensive) training sets yield more transferable force fields (but longer development time!)
- Things to include in training sets
 - Bond dissociation
 - Angle bending
 - Under/overcoordination
 - Key reactions, including transition states
 - Charges
 - Condensed phase data: Equations of state, heats of formation (experiment)

Bond energy

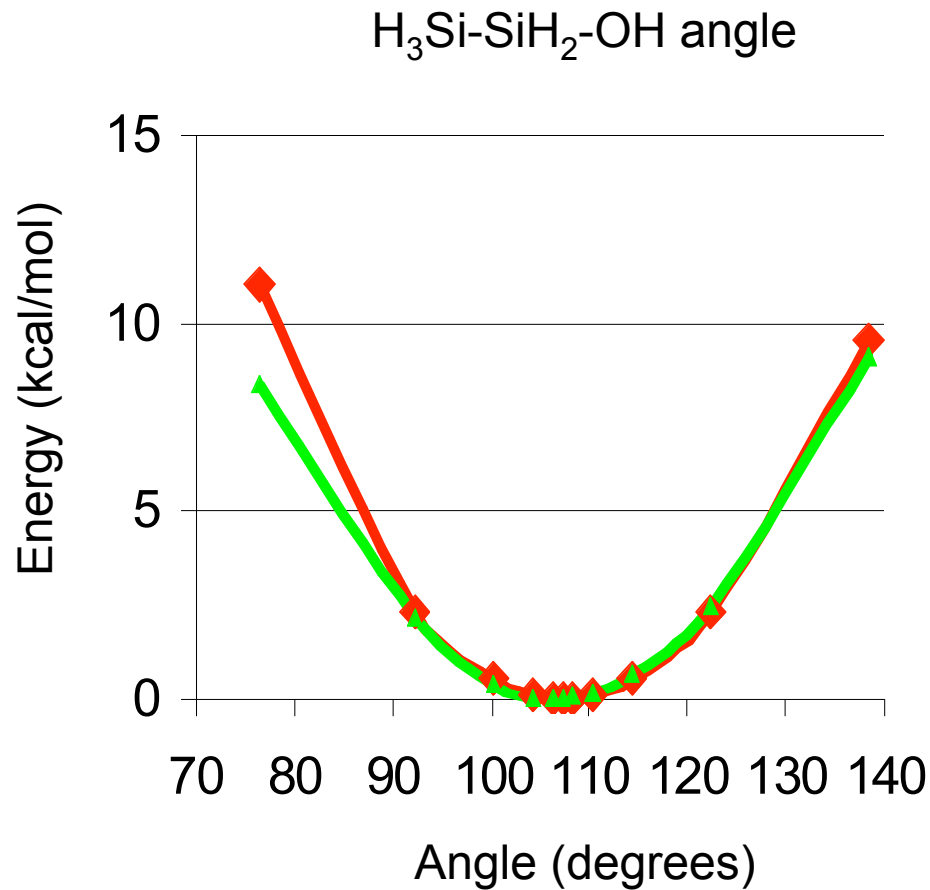


Other SiOH bonds:

- Si-Si
- Si=Si
- Si=O
- Si-H
- O-O
- O=O
- O-H

Valence angle bending

1. Individual valence angles

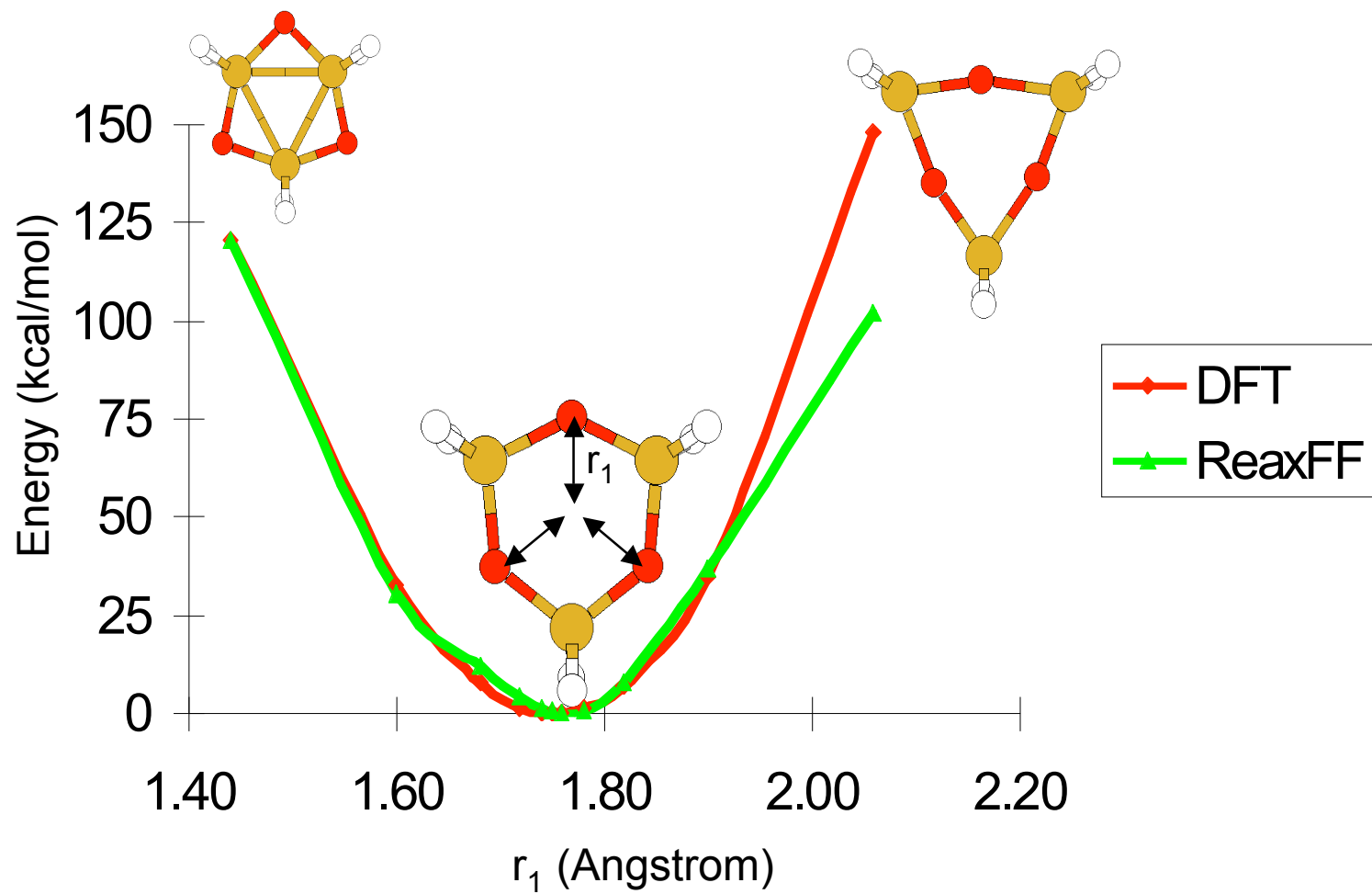


Other SiOH angles:

- | | |
|------------|-----------|
| - Si-Si-Si | - Si-Si-H |
| - Si-O-Si | - H-Si-H |
| - Si-Si-H | - H-O-H |
| - Si-O-H | - O-O-O |
| - O-Si-H | - Si-O-O |
| | - O-O-H |

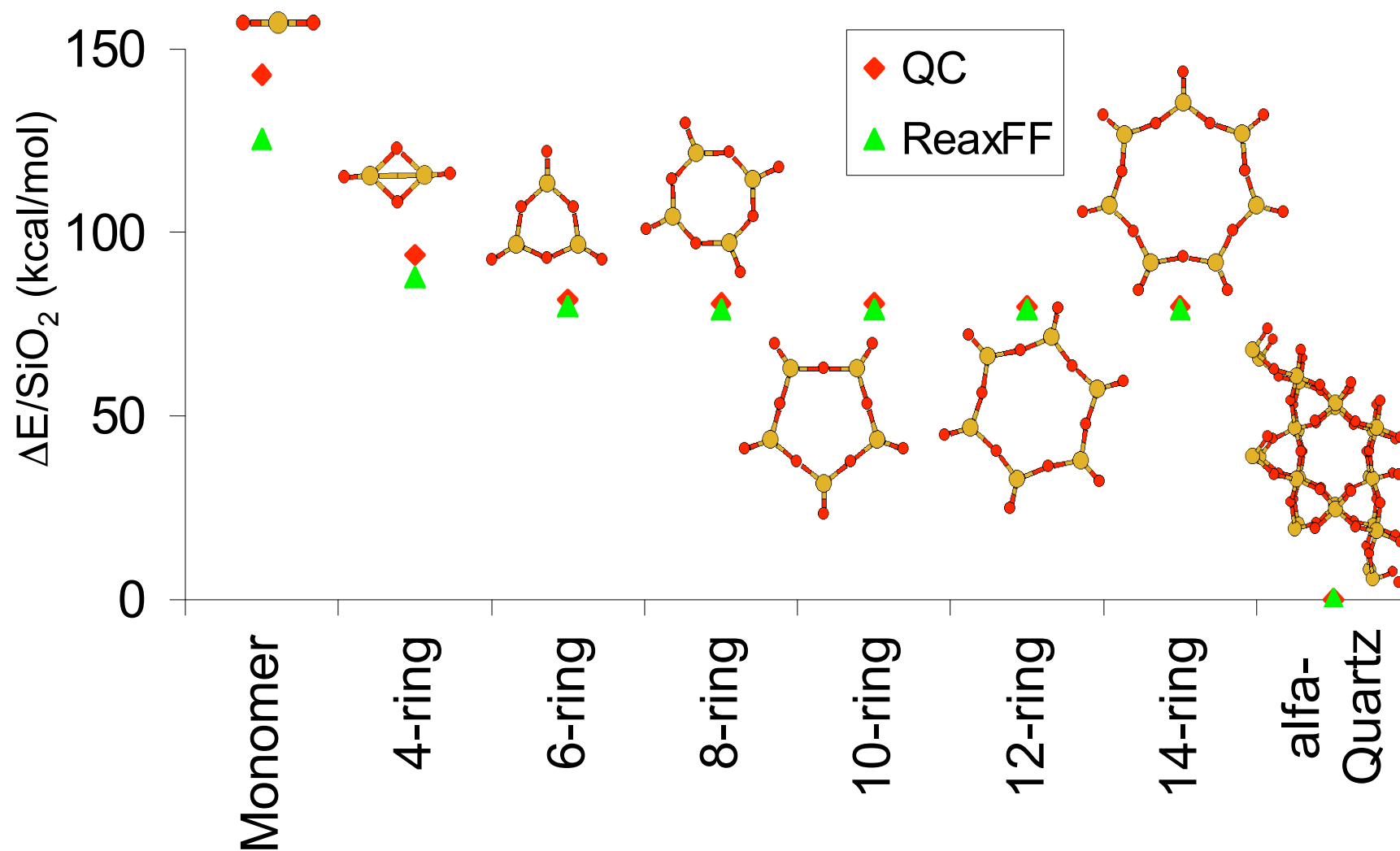
Valence angle bending

2. Ring deformation

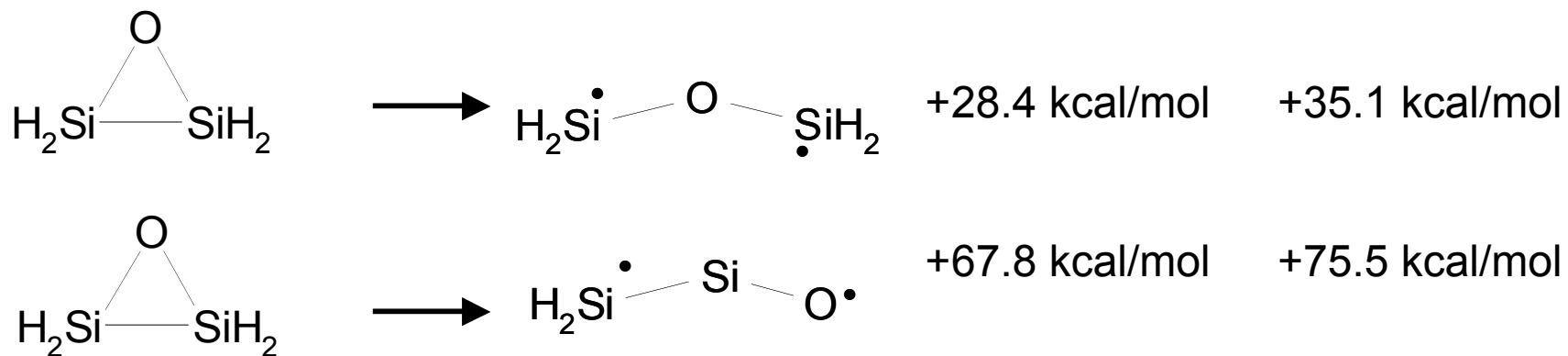
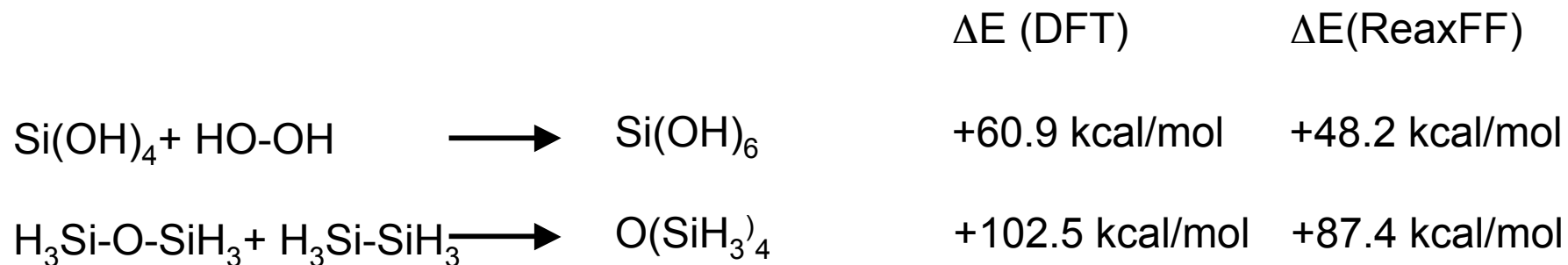


Valence angle bending

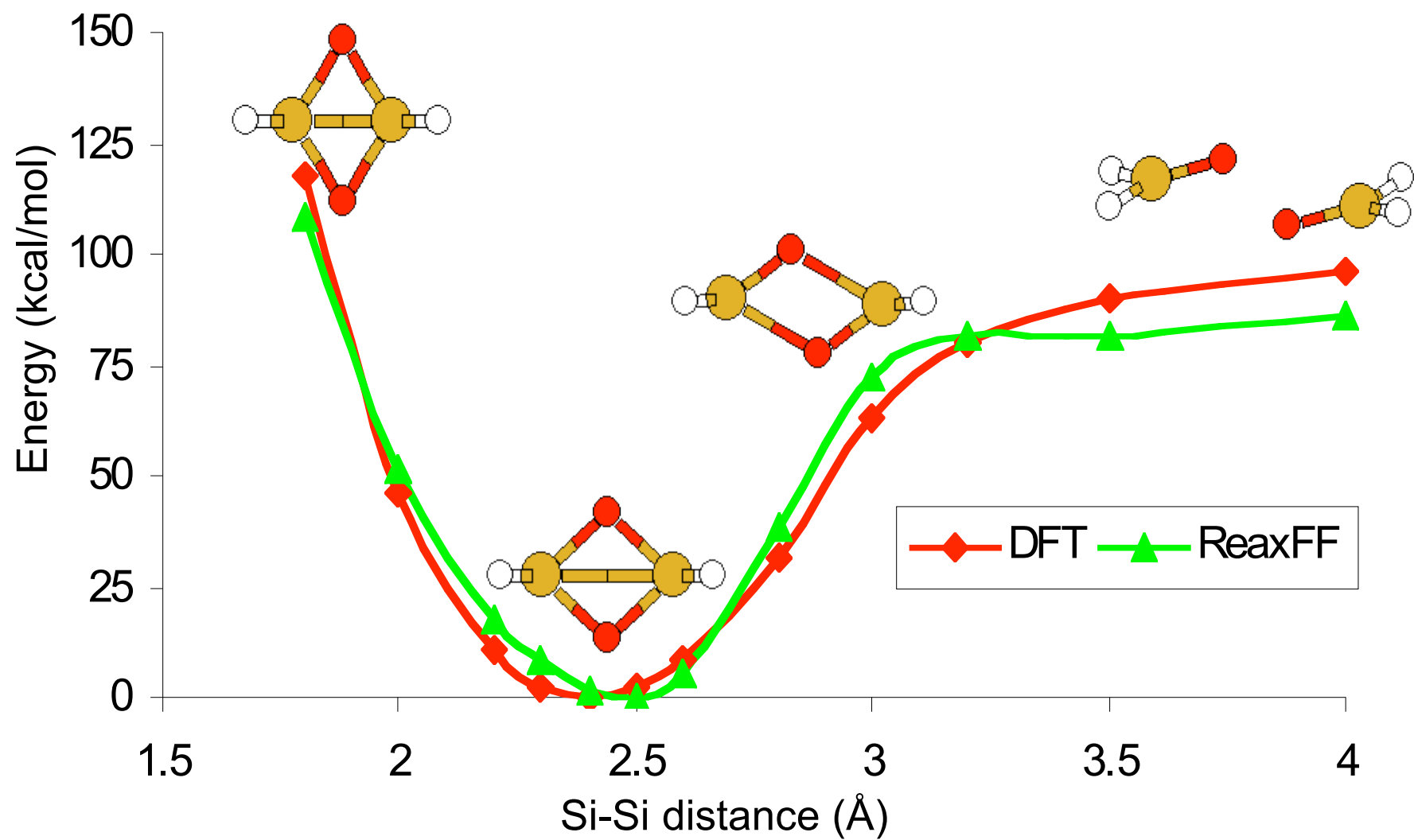
3. Ring size/ring strain



Over/undercoordination

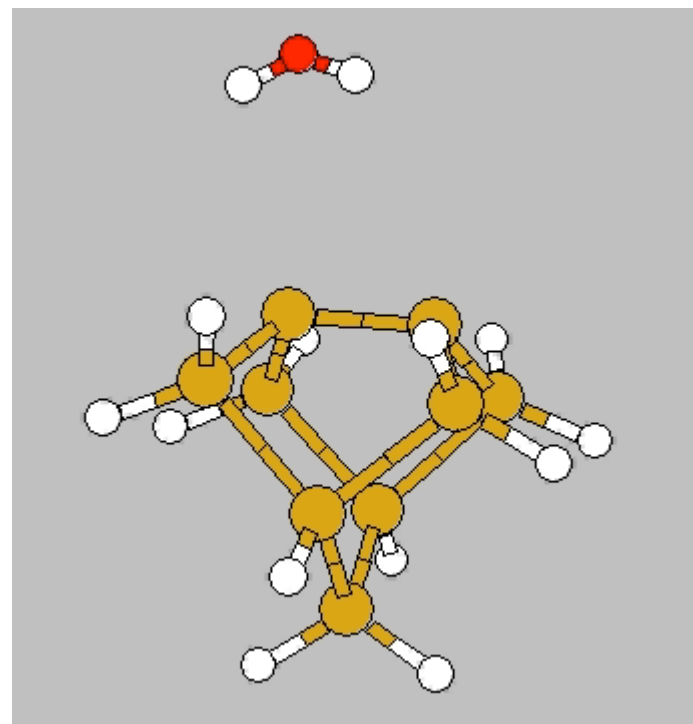
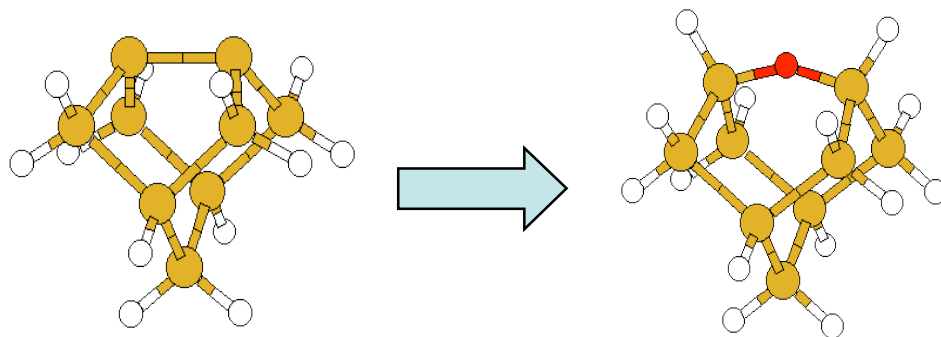
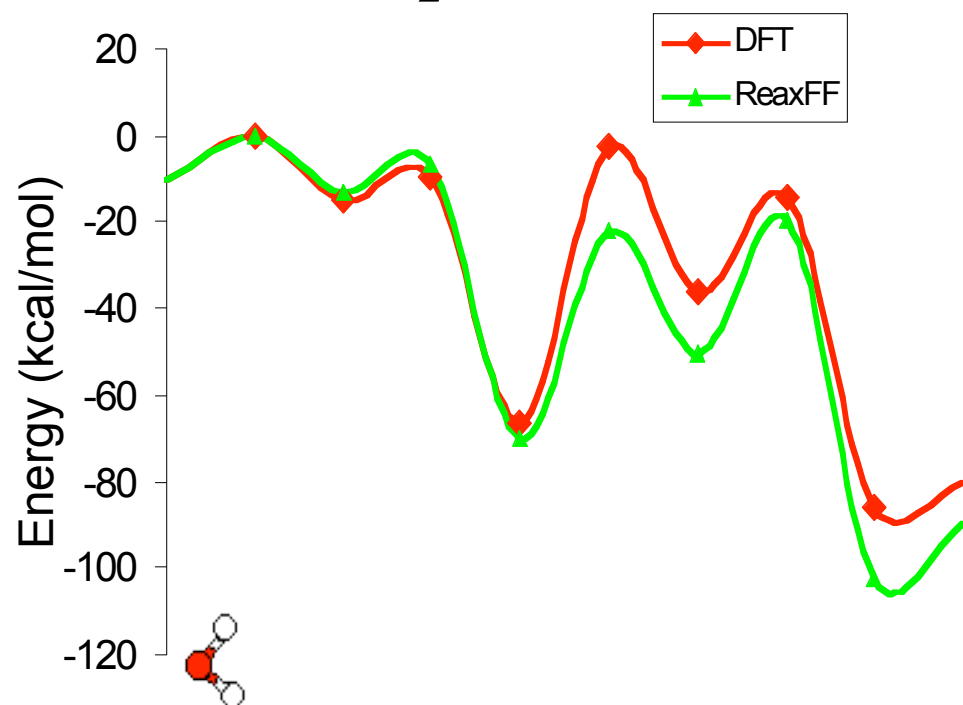


Reactions



Reactions

2. H₂O- incorporation in a Si-cluster

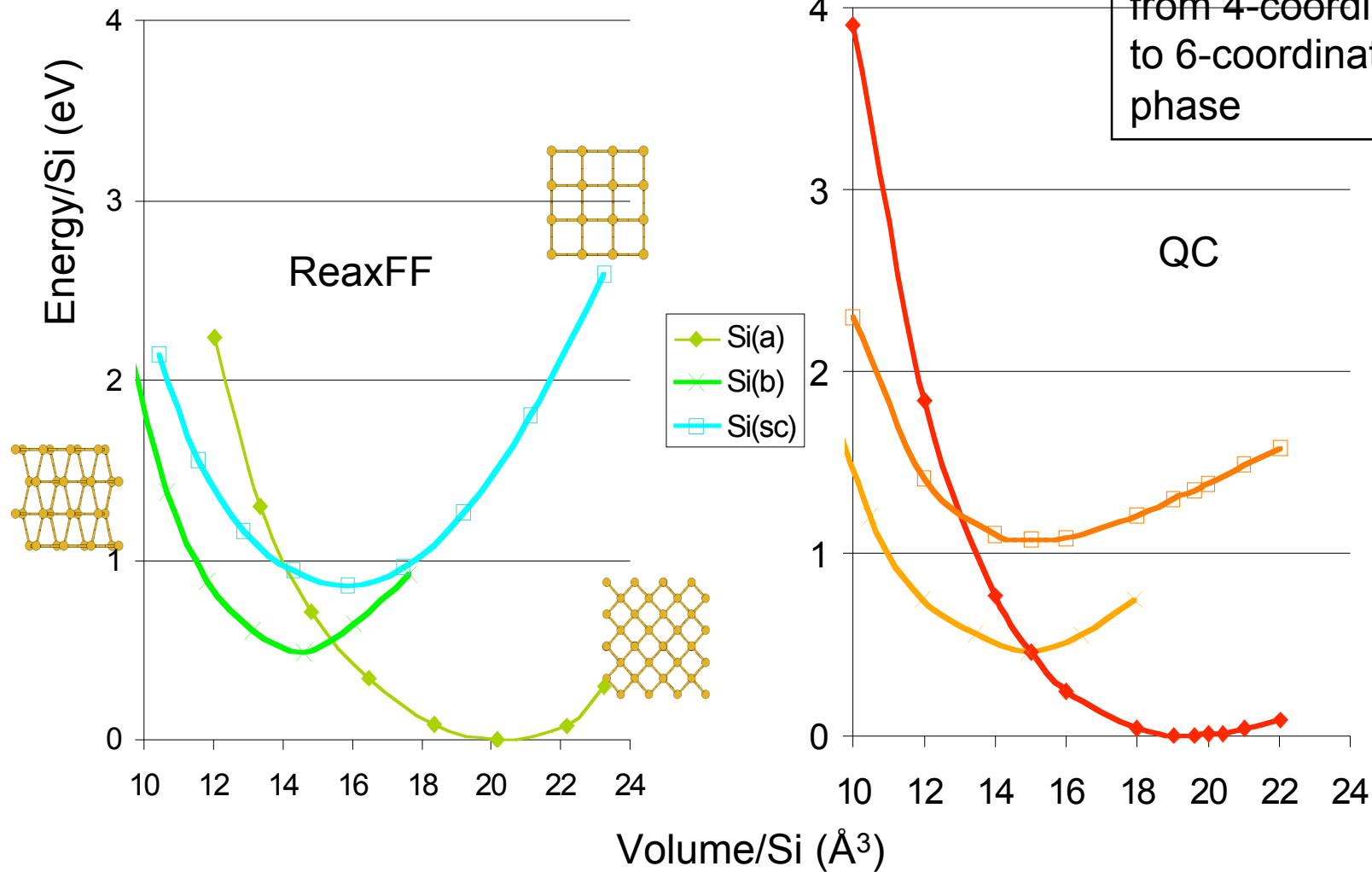


- Reactive force field can be used to simulate the entire reaction pathway

Equations of state crystals

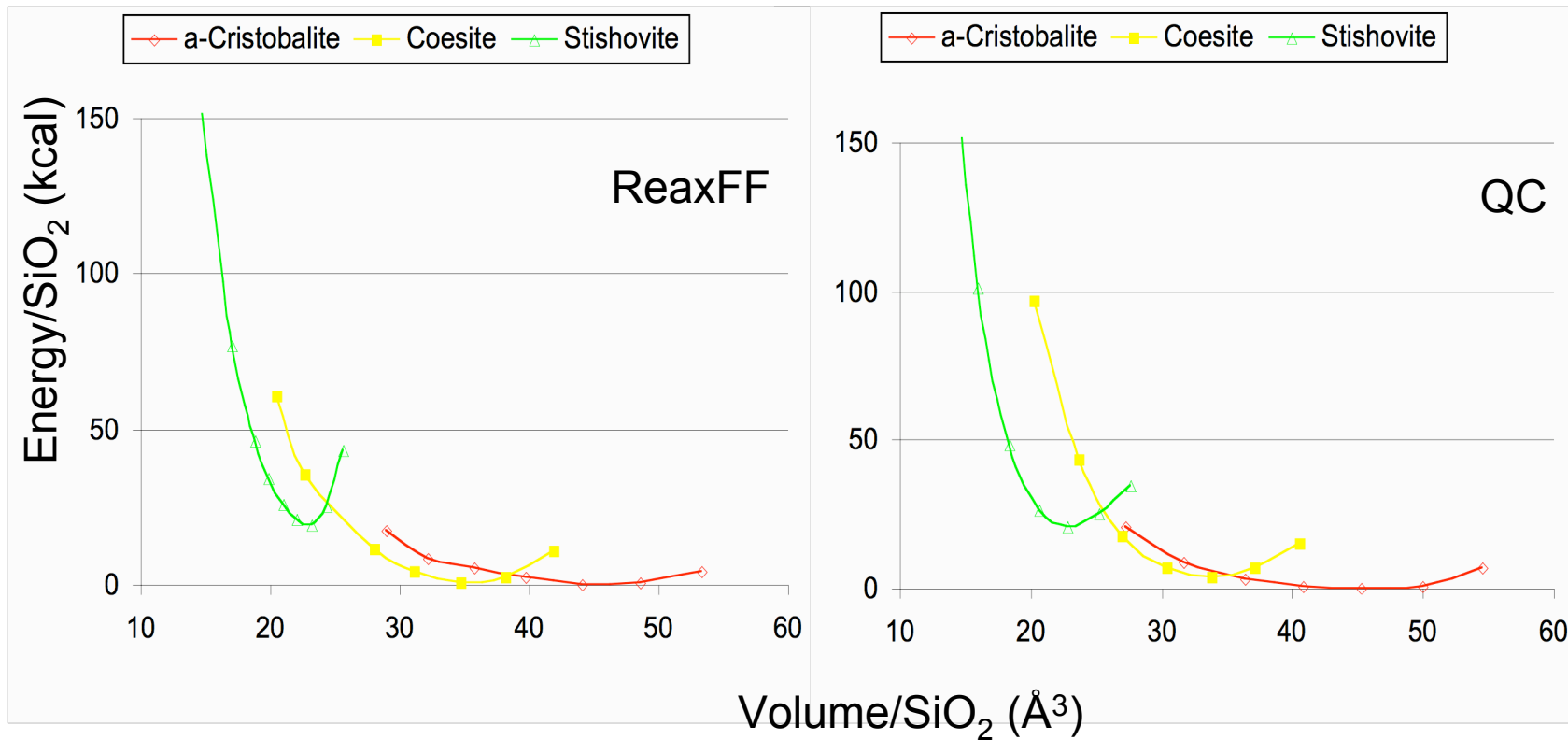
1. All-Si crystals

- Force field recognizes high-pressure transition from 4-coordinated (α) to 6-coordinated (β) phase



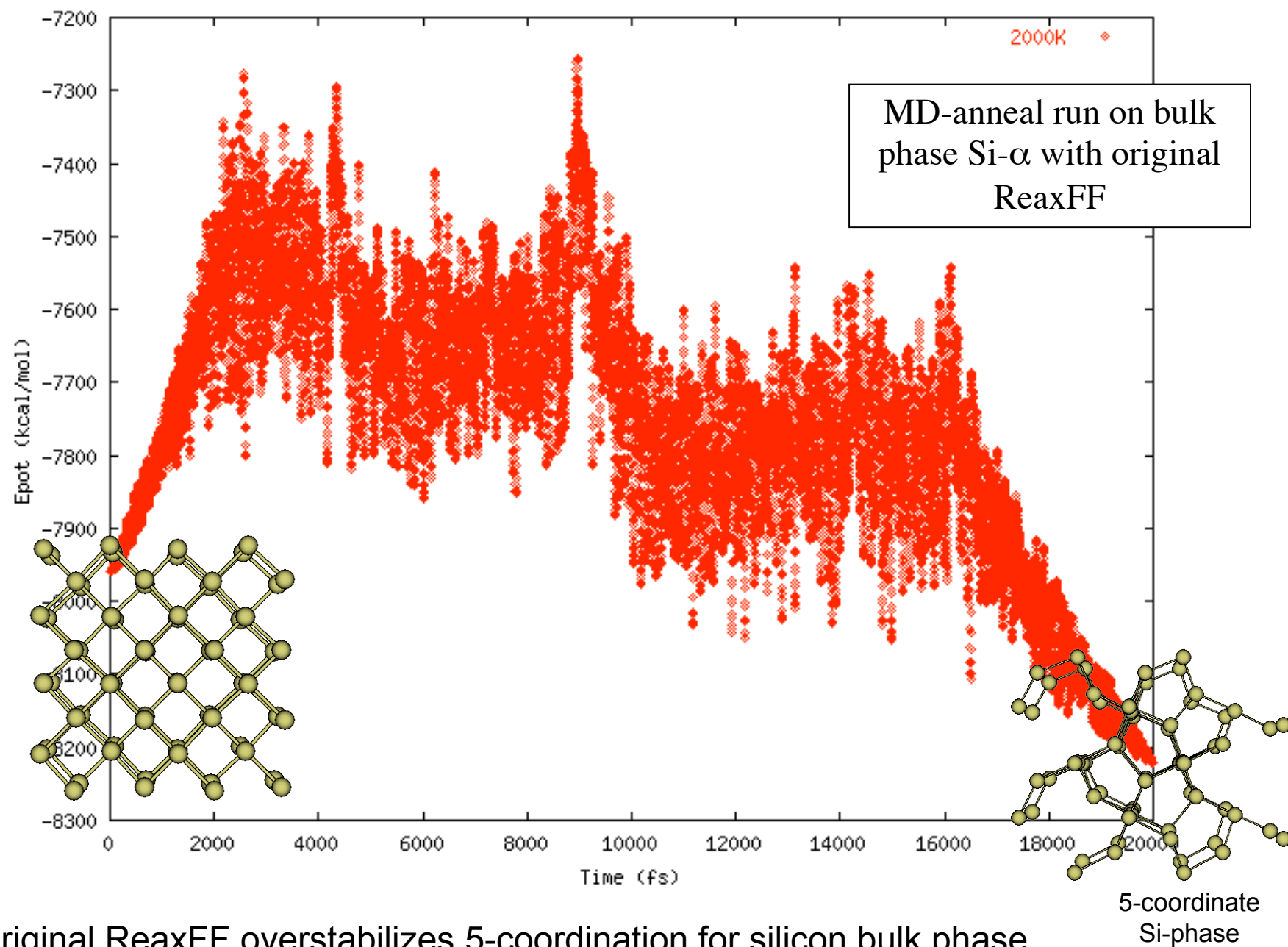
Compression/expansion crystals

2. Silicon oxide crystals



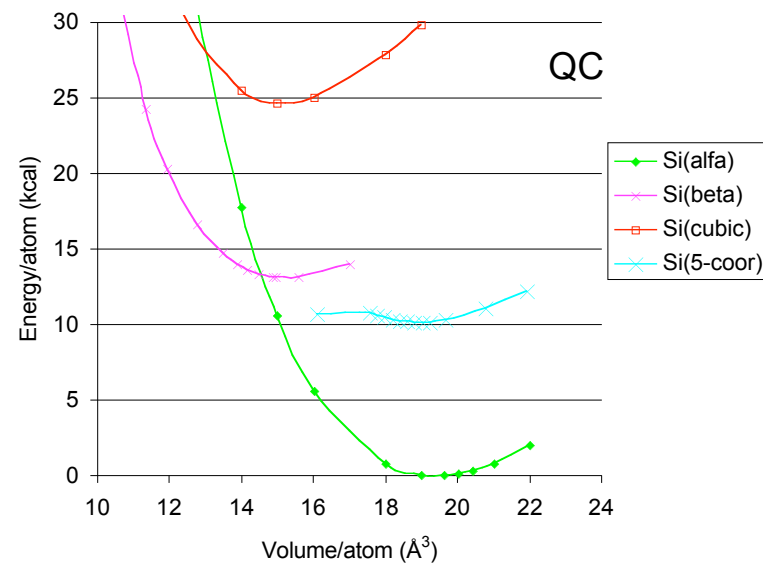
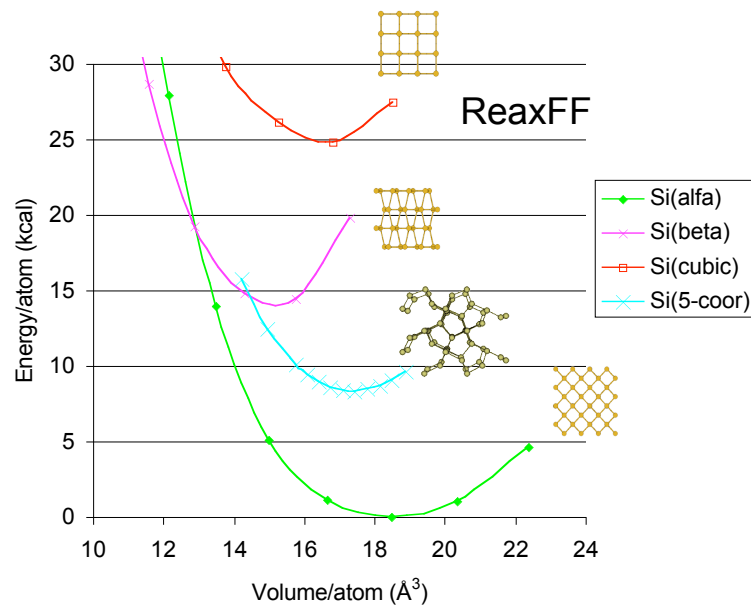
- ReaxFF reproduces the QC-data for both the clusters as well as the condensed phases.

Correcting a 'finished' ReaxFF force field



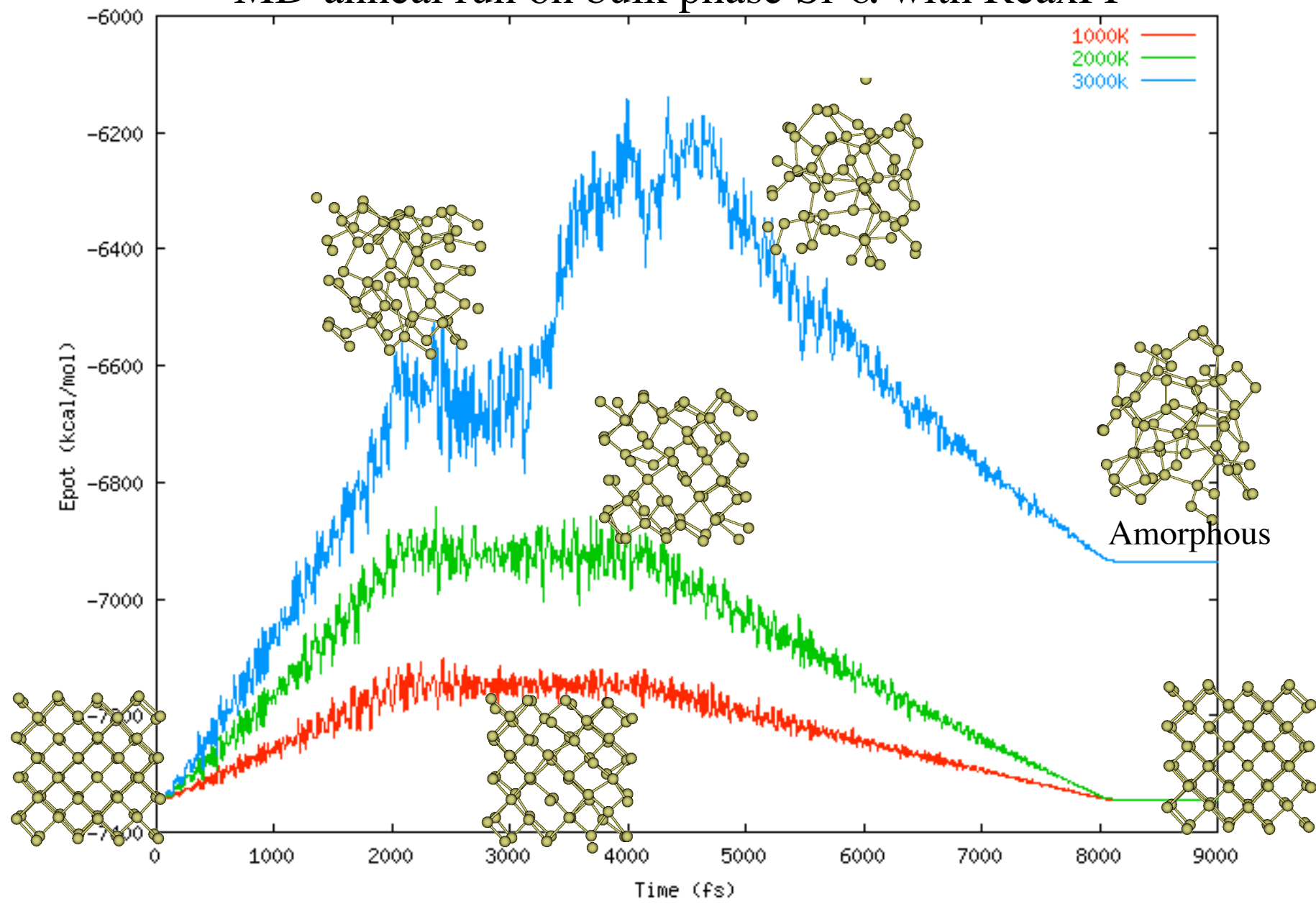
- Original ReaxFF overstabilizes 5-coordination for silicon bulk phase

Re-optimize ReaxFF with equation of state for 5-coordinate Si-phase



- Re-optimized ReaxFF gets proper stability for 5-coordinate Si-phase
- 5-coordinate phase is more stable than 6-coordinate Si(β) !
- 5-coordinate Si might be important in amorphous Si

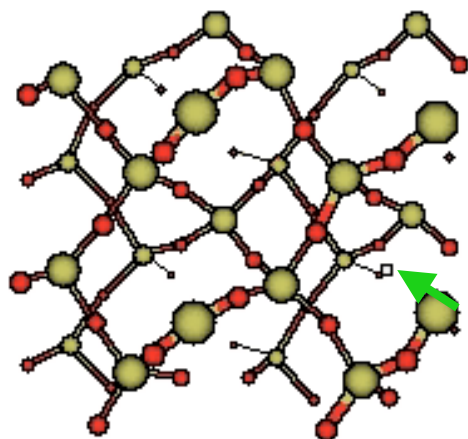
MD-anneal run on bulk phase Si- α with ReaxFF



Applications of the Reax Si/SiO force field

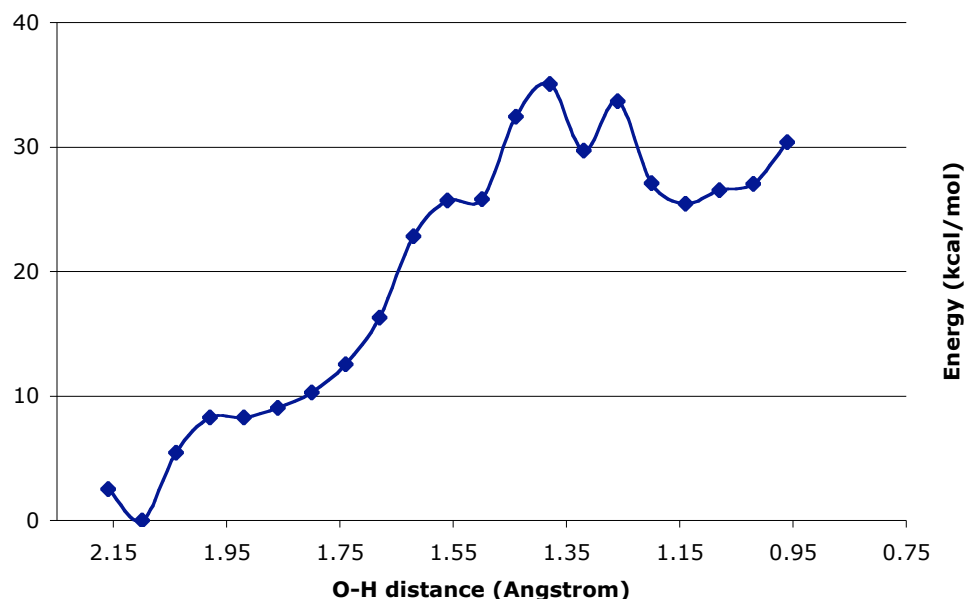
- Hydrogen diffusion in Si/SiO₂ interfaces
- Stability of PDMS polymers

ReaxFF simulations on H-diffusion and bonding in α -quartz



Hydrogen radical in
72-atom α -quartz
T=100K; reaction enforced
by a moving restraint

ReaxFF



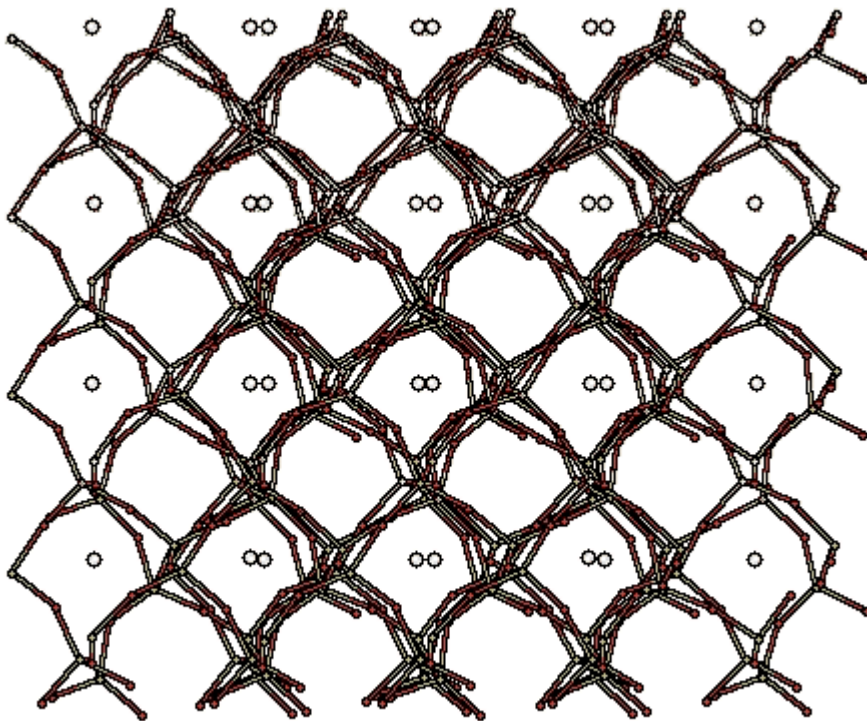
Seqquest:

$$E(\text{quartz_H}) - E(\text{quartz} + \text{H}) = +24 \text{ kcal/mol}$$

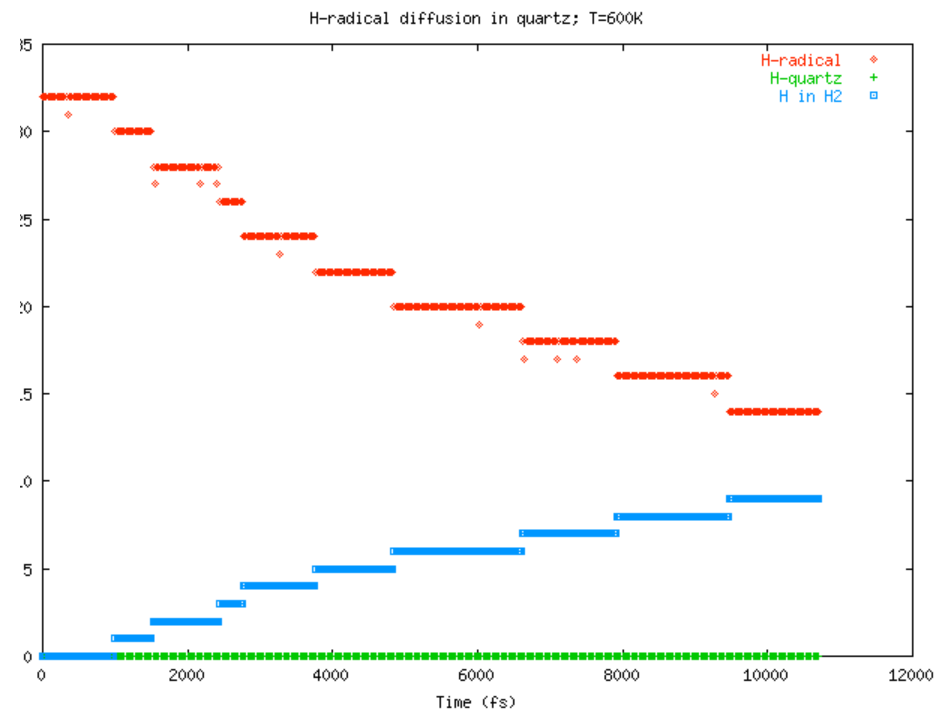
-Good agreement between Reax
and SeqQuest reaction energies

ReaxFF simulations on H-radical diffusion through α -quartz

T=600K



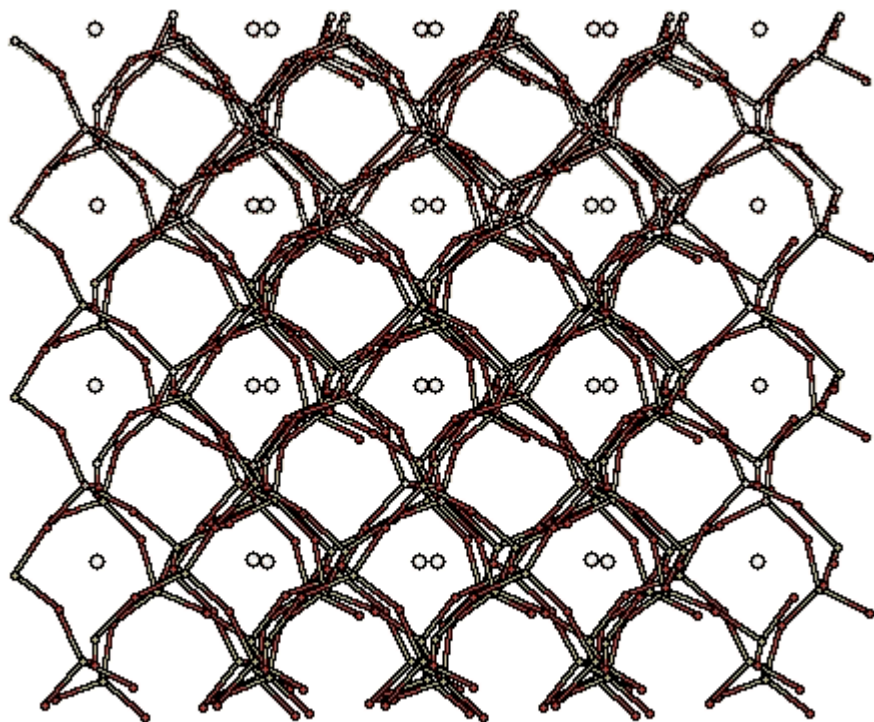
32 H-radicals in 576-atom α -quartz system



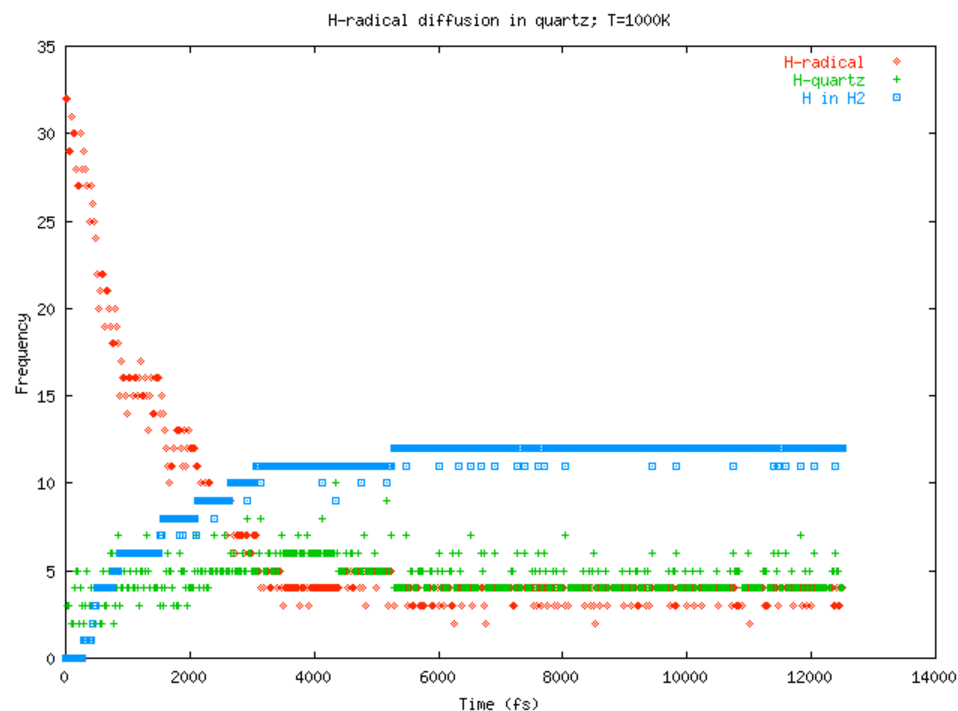
No reaction of H-radicals with lattice oxygens; all H-radicals diffuse and form H₂

ReaxFF simulations on H-radical diffusion through α -quartz

$T=1000\text{K}$



32 H-radicals in 576-atom α -quartz system




-Elevated temperatures result in H-reaction with lattice oxygens.
H₂ formation still dominates

Conclusions

- ReaxFF has proven to be transferable to a wide range of materials and can handle both complex chemistry and chemical diversity. Specifically, ReaxFF can describe covalent, metallic and ionic materials and interactions between these material types.
- The low computational cost of ReaxFF (compared to QM) makes the method suitable for simulating reaction dynamics for large ($>> 1000$ atoms) systems (single processor). ReaxFF has now been parallelized, allowing reactive simulations on $>> 1000,000$ atoms.

group	1*	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
period	Ia	IIa	IIIa**	IVa	Va	VIa	VIIa	VIIIa	VIIIa	VIIIa	Ib	IIb	IIIb	IVb	Vb	VIb	VIIb	VIIIb
1	H	He																
2	Li	Be																
3	Na	Mg																
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Ac															

 : not currently described by ReaxFF