Atom-Atom Potentials

A study of self-assembling
molecular rotors on a metal surface

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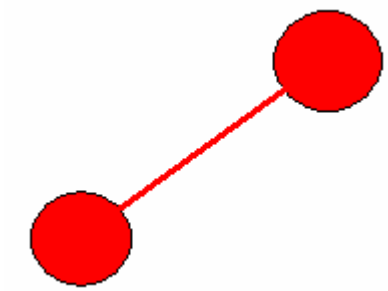
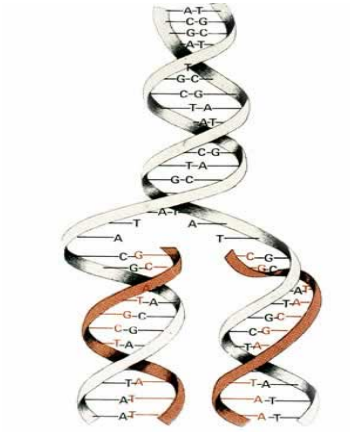
Big Picture

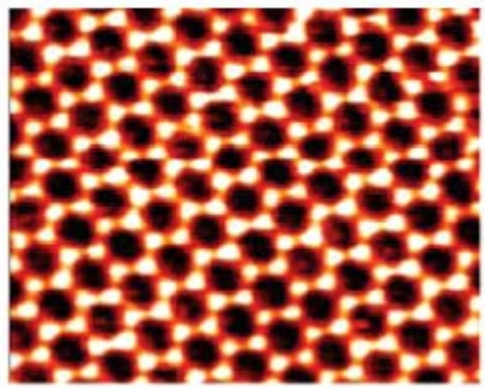
- Molecular rotors on a lattice –



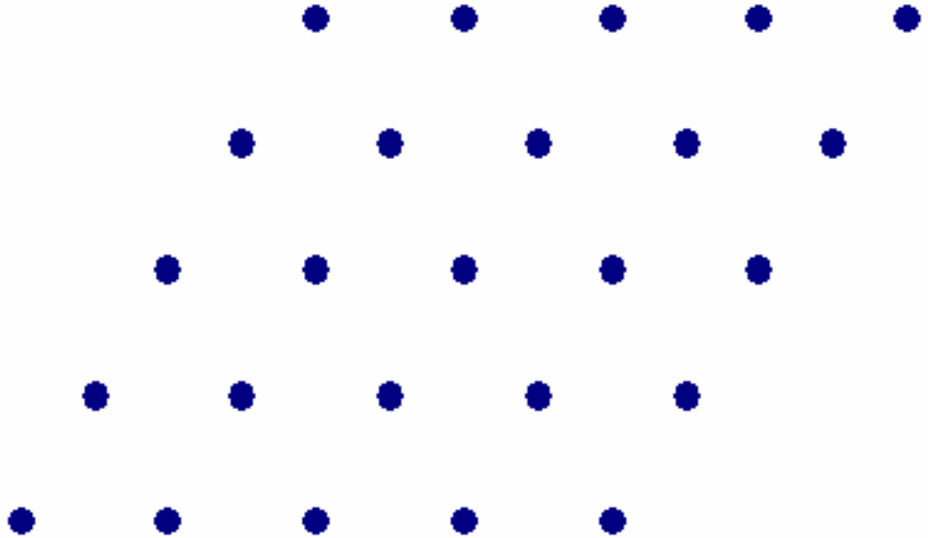
- Self Assembly –



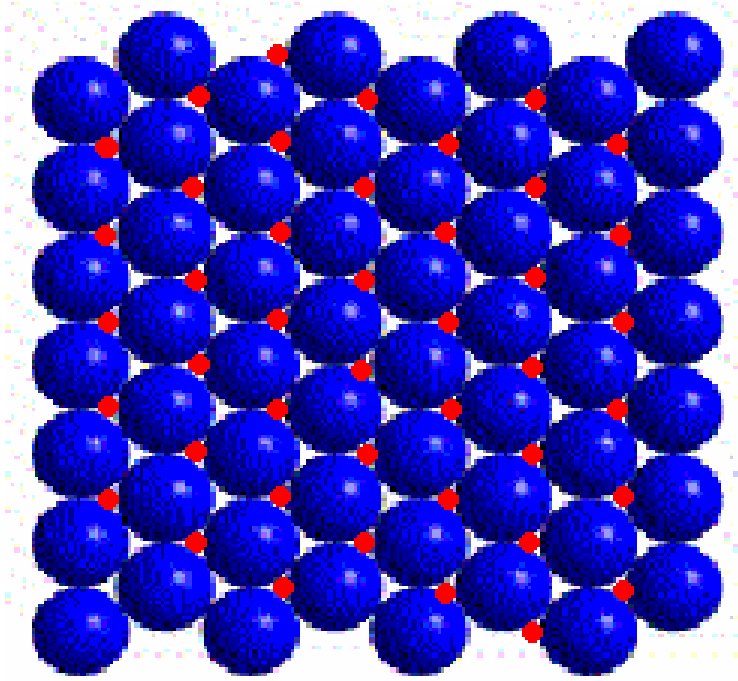
- Patterns/Clusters -



Lattice Concepts

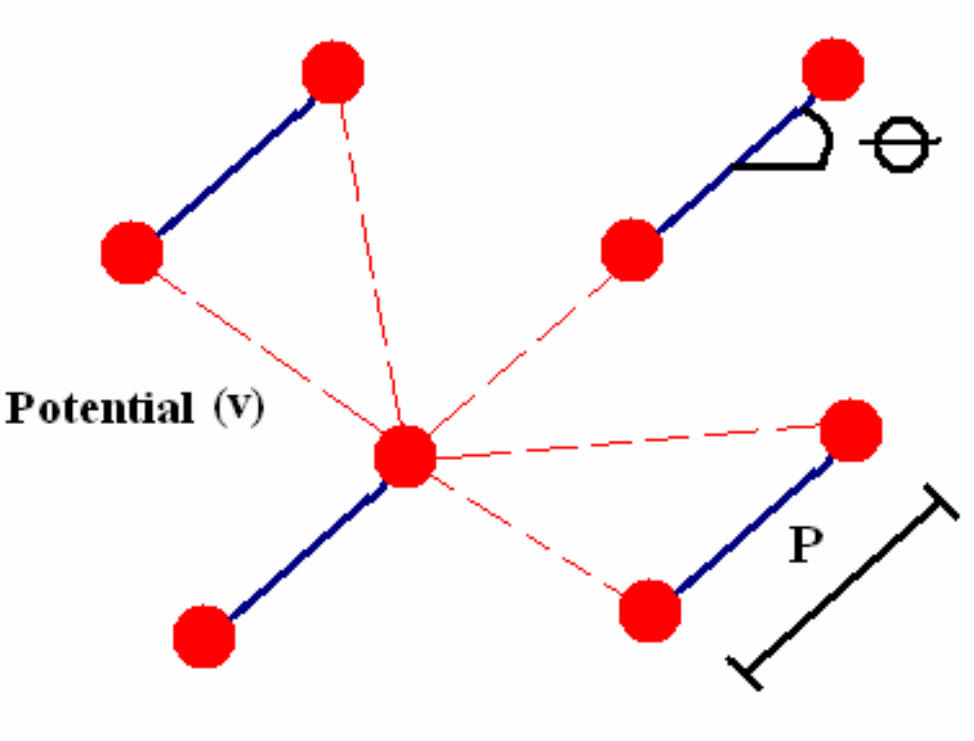


Hexagonal Lattice



Gold Surface

Molecular Rotors

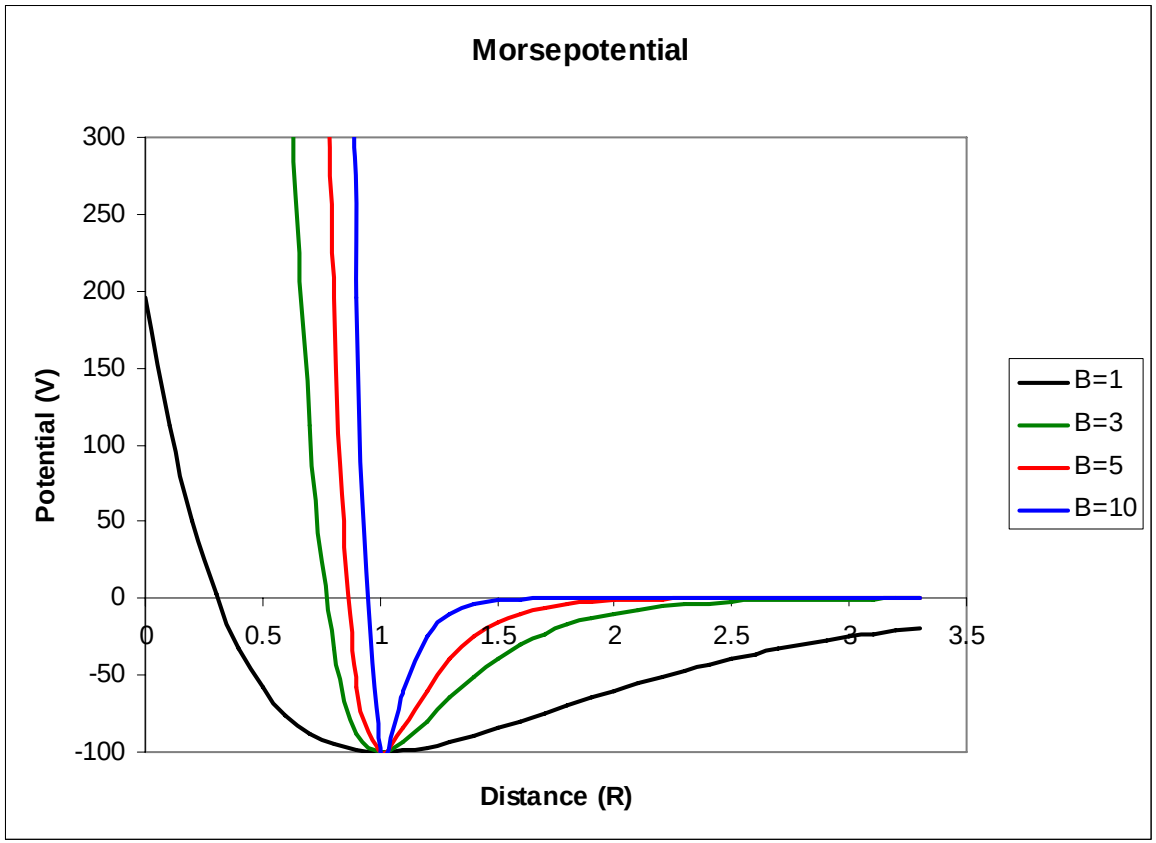


Properties-

- Theta
- Length (P)
- Potential (V)

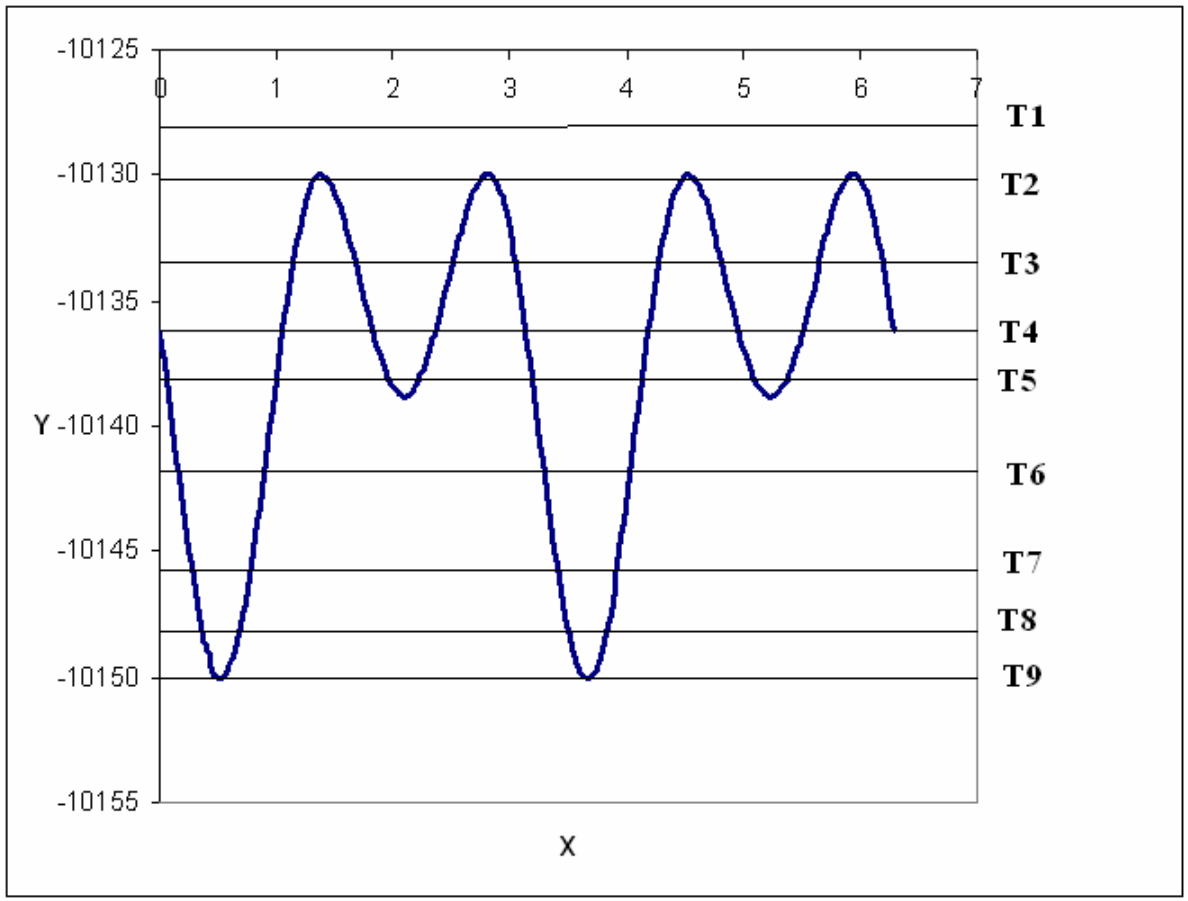
Morse Potential

$$V = D * e^{-B(R-\mathrm{Re})} * (e^{-B(R-\mathrm{Re})} - 2)$$

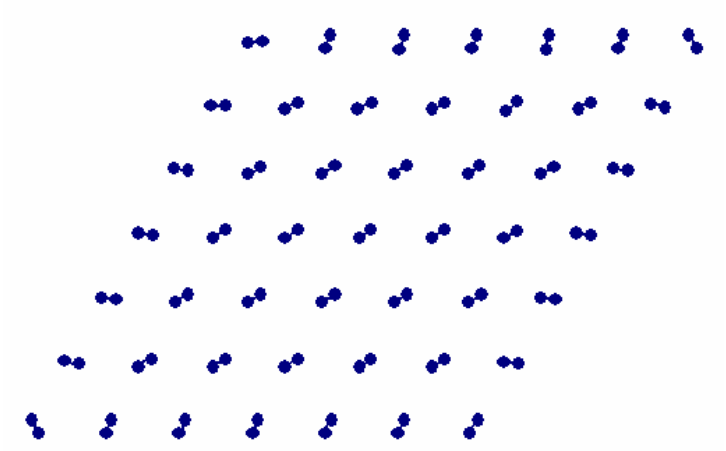


Search Methods

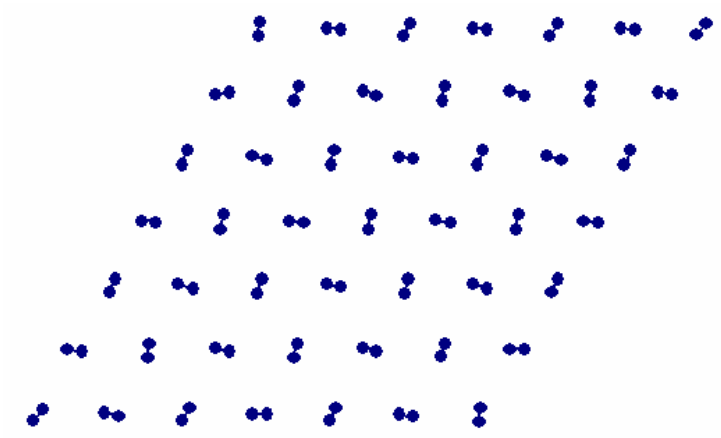
- Threshold Acceptance



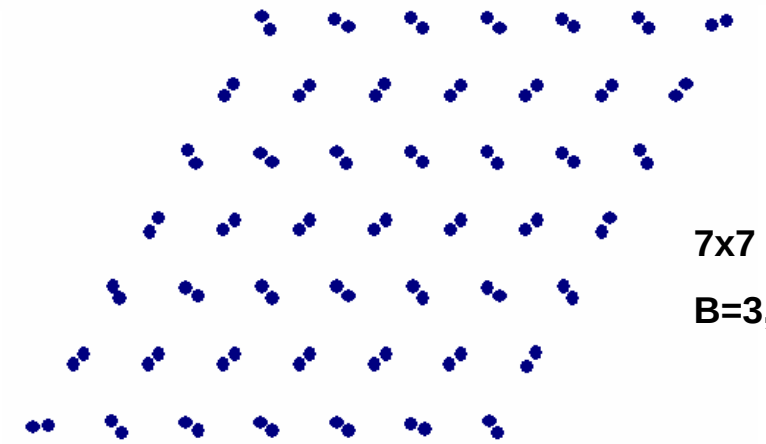
Patterns



7x7 hexagon lattice
B=1, Re=.8, P=.2



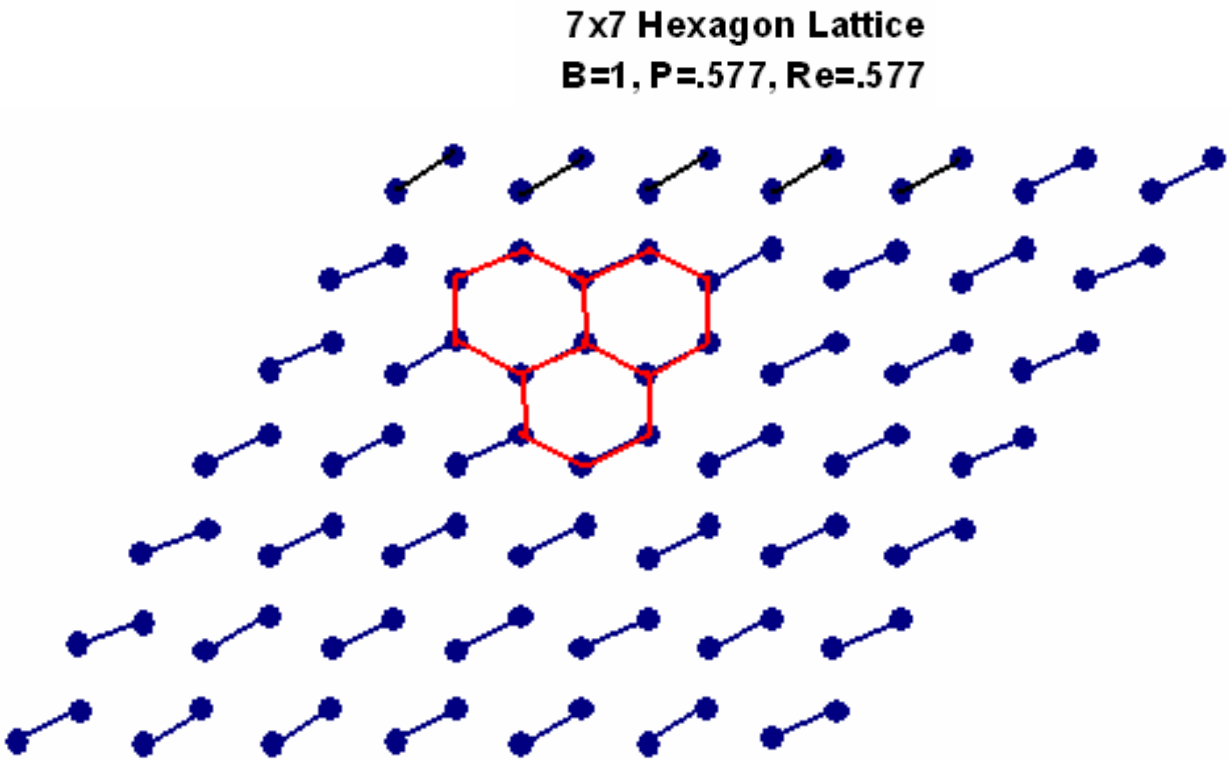
7x7 hexagon lattice
B=5, Re=.8, P=.2



7x7 hexagon lattice

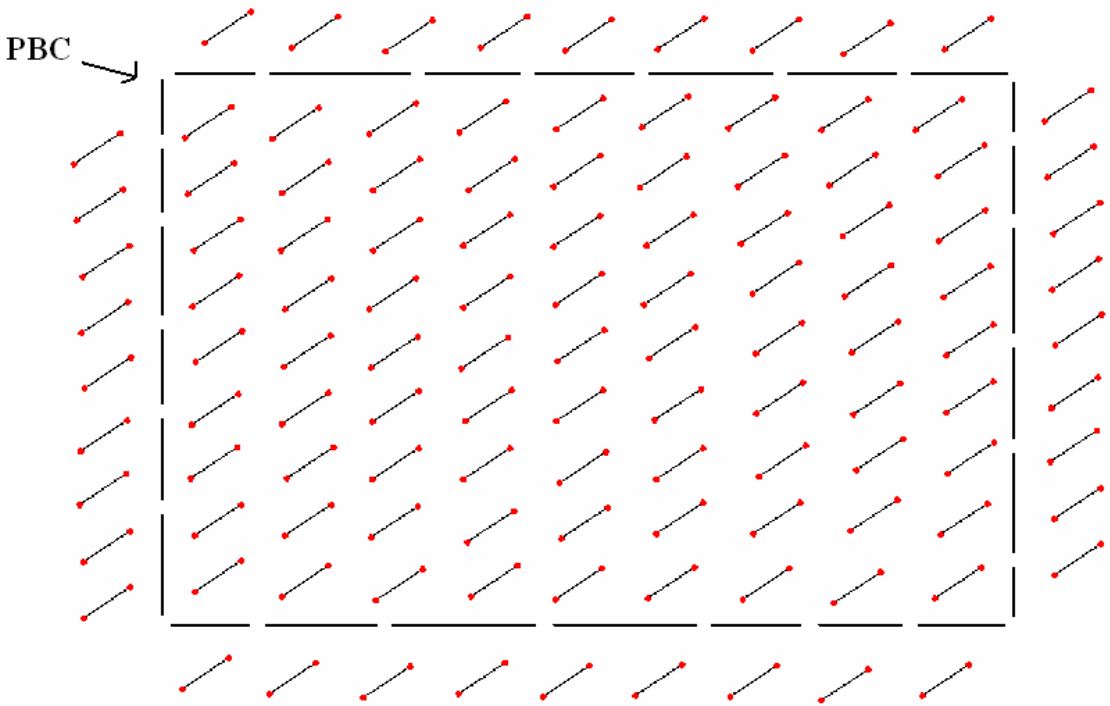
B=3, Re=.8, P=.2

Honeycomb Pattern



- Repeating Hexagons form honey comb structure
- Rotor length is equal to Re as well as distance between adjacent rotor points

Focusing our future work

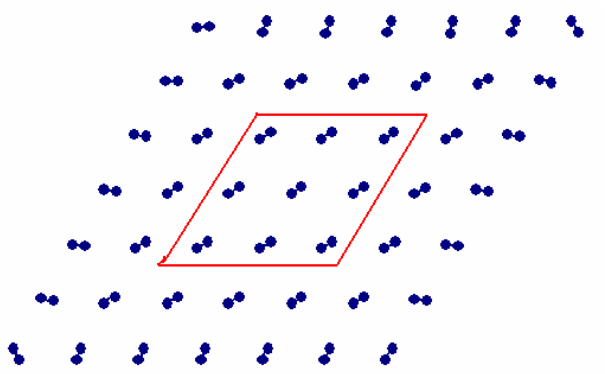


Periodic Boundary Conditions (PBC)

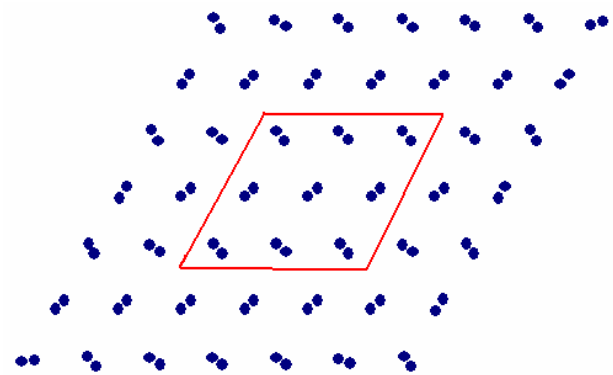
- Finite vs. Infinite Lattice

Focusing our future work

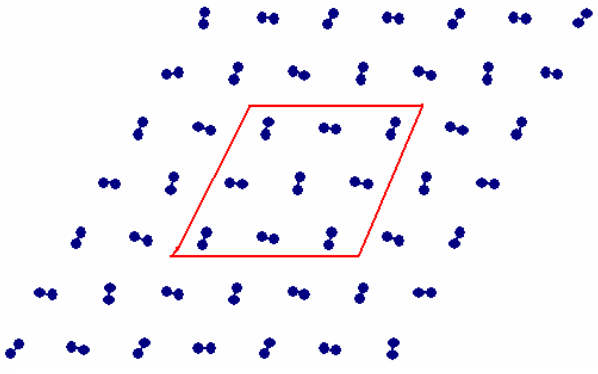
- Assume patterns exist



(1x1) pattern



(1x2) pattern



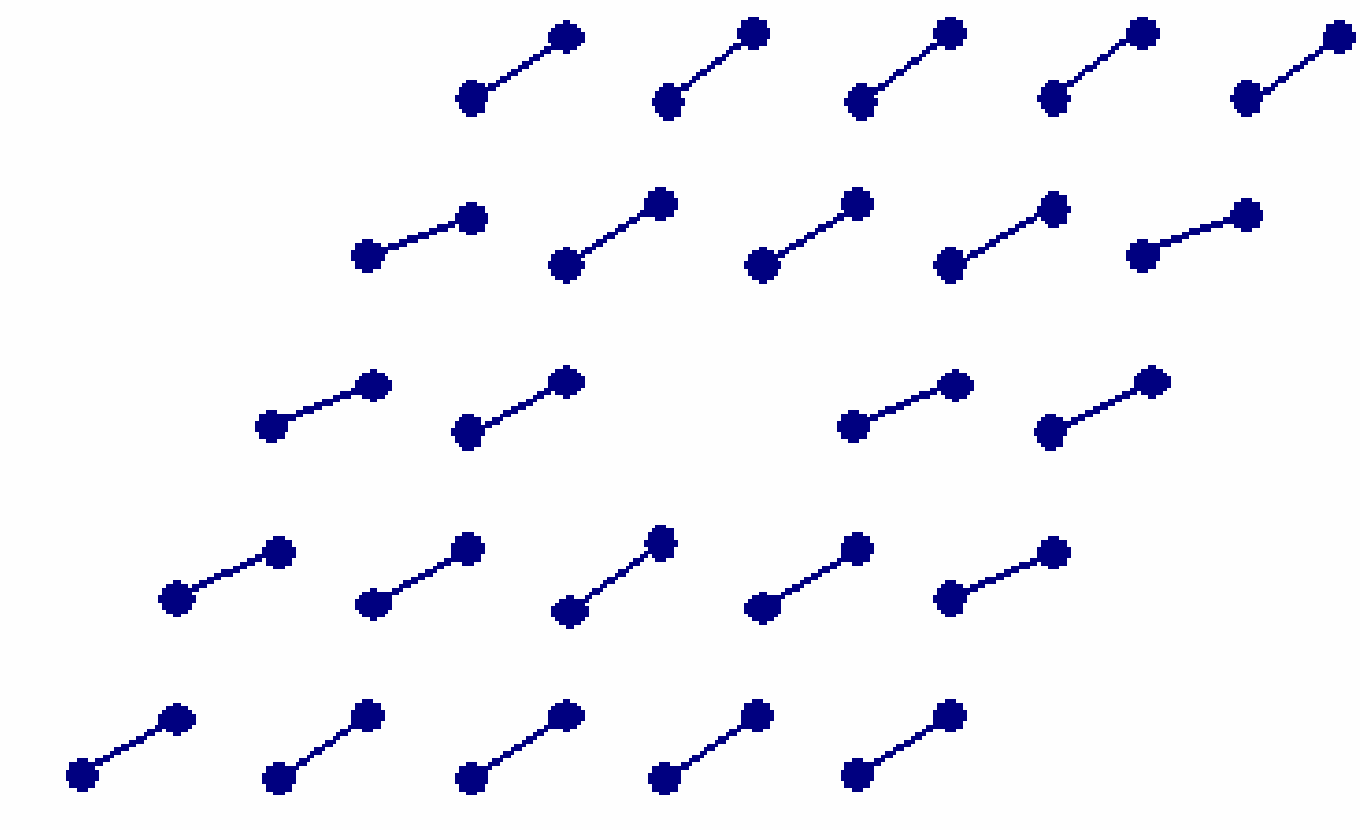
(2x2) pattern

- Back to the big picture

Defects

5x5 Hexagon Lattice

B=1, P=.577, Re=.577



Questions