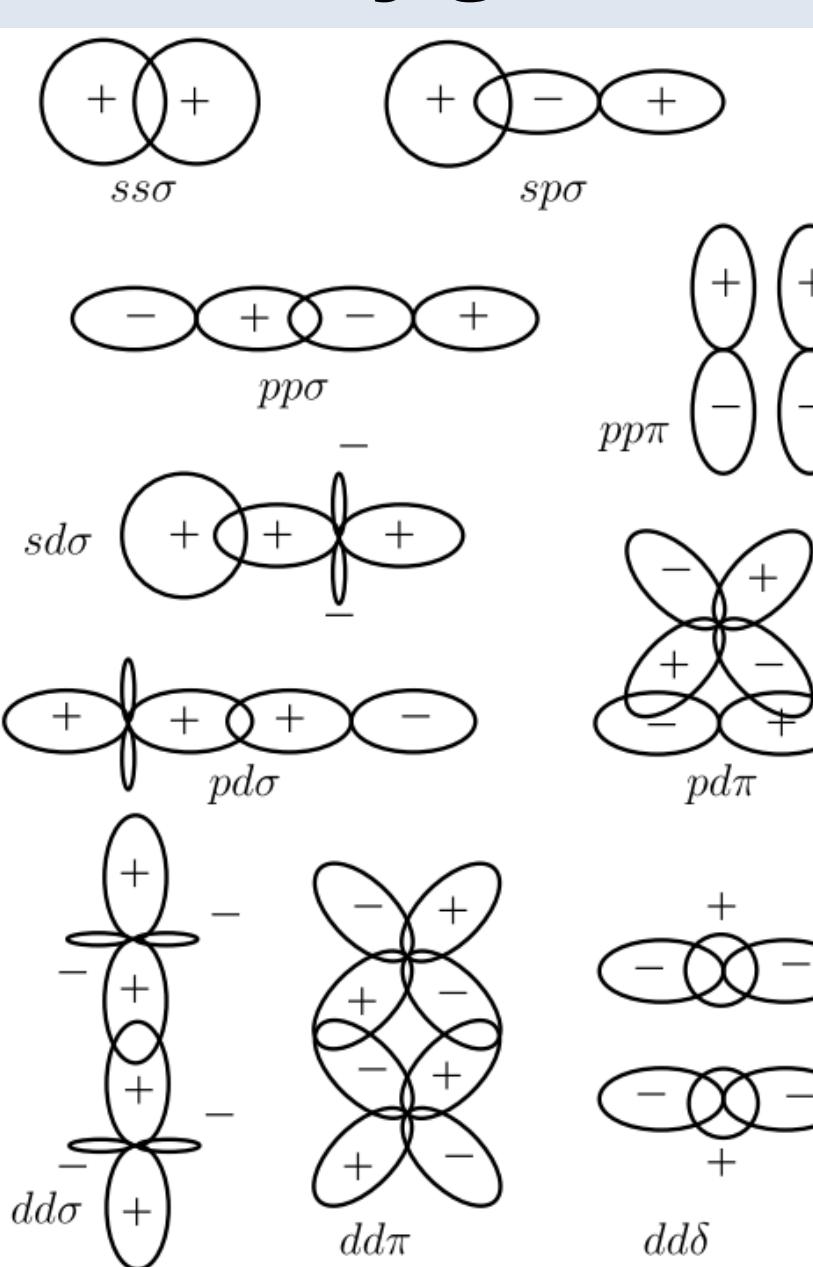


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## Screw dislocations control plasticity in titanium.

- Solute-hardening is not well understood on an atomistic scale.*
- Ab initio quantum mechanics is too computationally expensive.*
- Tight-binding approximation is quantum mechanical yet less expensive.*
- We have made a tight-binding model for titanium with which we can investigate atomistic mechanisms for oxygen solute-hardening.*



## Tight-binding models need parameters.

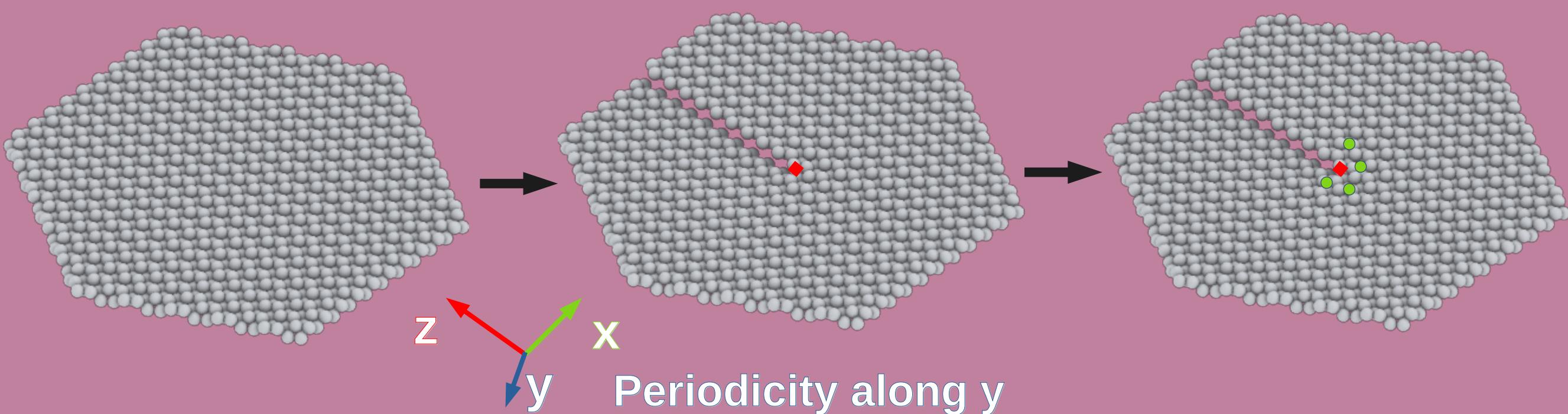
- Overlaps between atomic orbitals of atoms are parameters.
- This titanium model is d-orbital only.
- Ab initio Density Functional Theory (DFT) calculations and empirical quantities are fitted to.
- Particle swarm algorithm used for fitting.
- Validation achieved by comparison of:
  - Lattice wave dispersion (phonons).
  - Generalised stacking fault energy surfaces.
  - Dislocation core structure.
  - Dissolution/vacancy formation energies.

## Results of Fitting

Quantity	Units	TB model	Target
$a_\alpha$	[bohr]	5.52	5.57
c/a	ratio	1.571	1.587
$C_{11}$	[GPa]	175.3	176.1
$C_{33}$	[GPa]	195.5	190.5
$C_{44}$	[GPa]	59.6	50.8
$C_{12}$	[GPa]	70.2	86.9
$C_{13}$	[GPa]	67.5	68.3

## Method

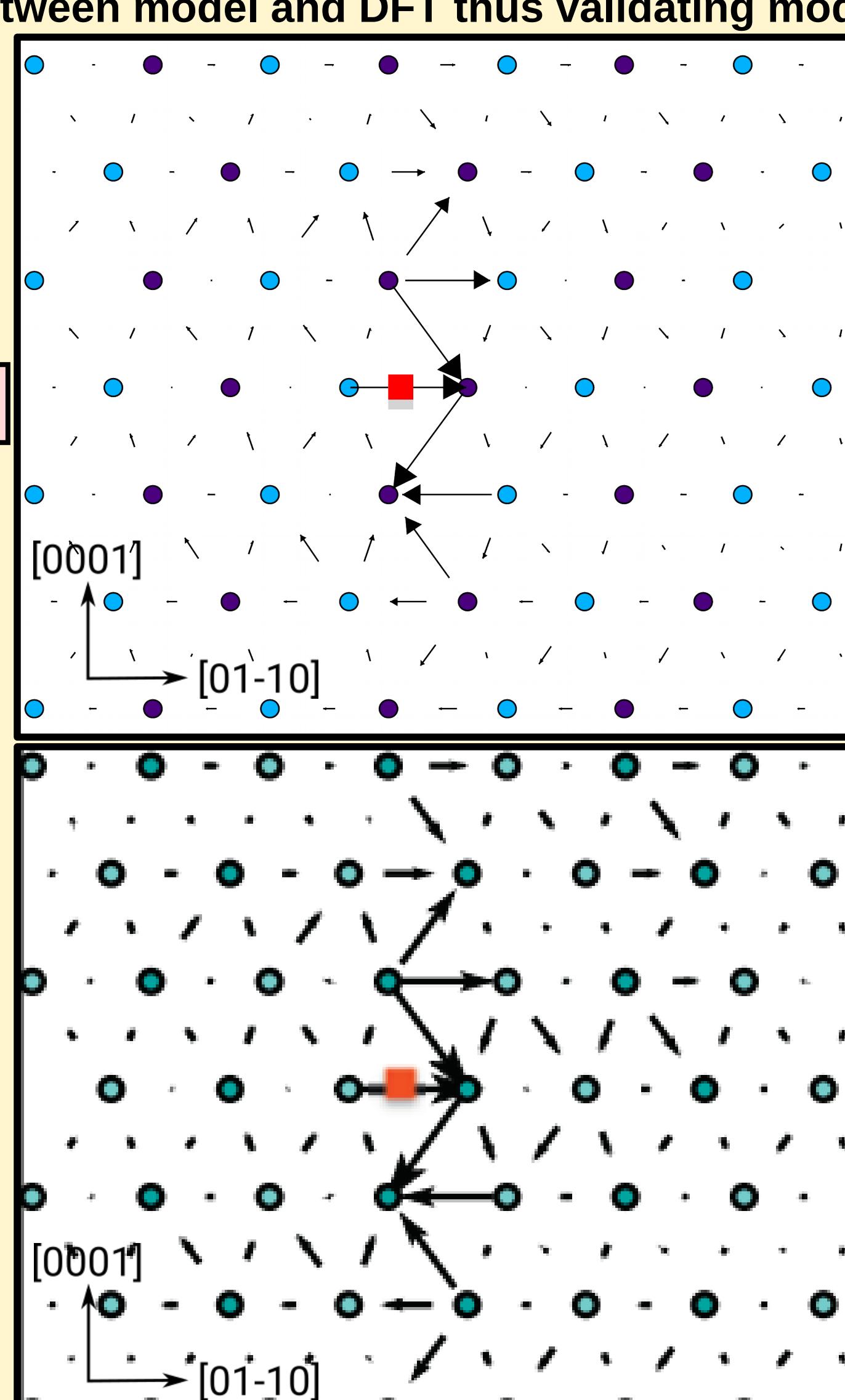
- Create dislocation in cell.
- Put oxygen into different sites (octahedral) near core.
- Relax cell to see how the core structure changes.



## Dislocation Core Structure

Differential Displacement maps of screw dislocation core upon relaxation in tight-binding (TB) and Density Functional Theory (DFT / ab initio).

- Arrows denote out-of-plane displacements.
- An arrow joining two columns corresponds to displacement by a full Burger's vector.
- Position of elastic centre of dislocation core is marked by the red square.
- Good agreement between model and DFT thus validating model.



DFT [1]

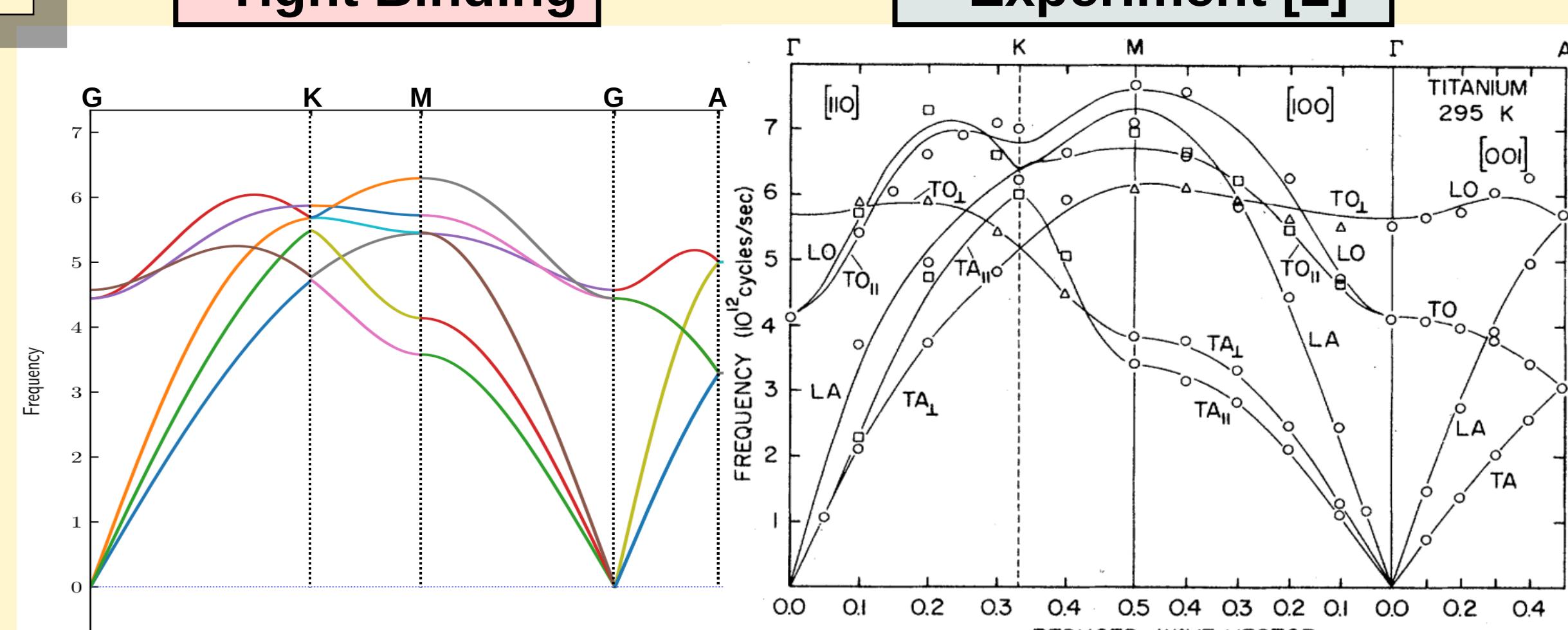
## Validation Tests

Quantity	Units	TB model	Literature
$E_{\text{vacancy formation}}$	[eV]	1.01	1.27 [Exp. Hashimoto (1984)] 1.95 [DFT Angsten (2013)]
$\Delta E_{\text{solution}}$ (tetra. - octa.)	[eV]	0.80	1.20 [DFT Kwasniak (2013)]

### Phonons

### Tight Binding

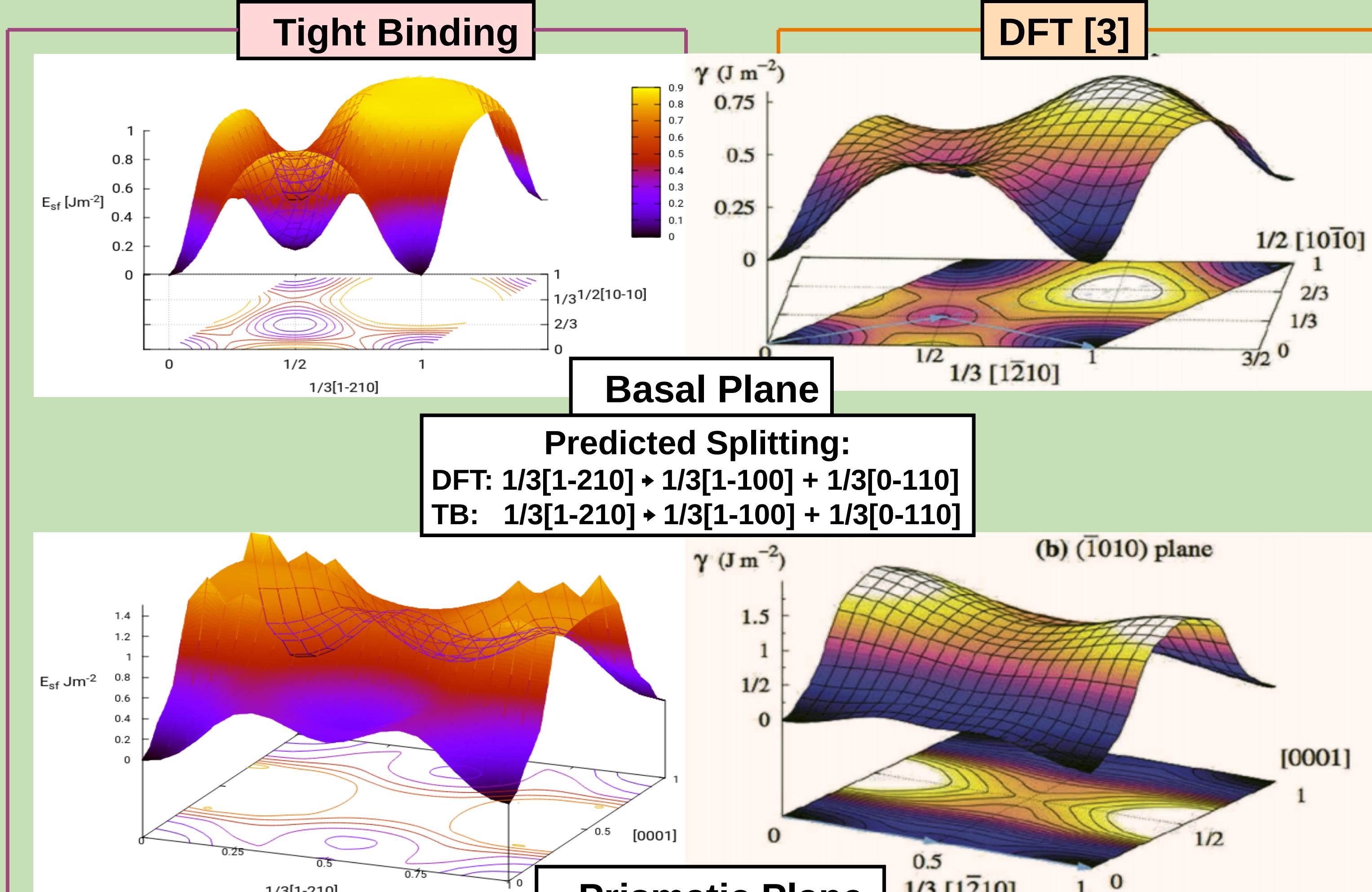
### Experiment [2]



## Generalised Stacking Fault Energies

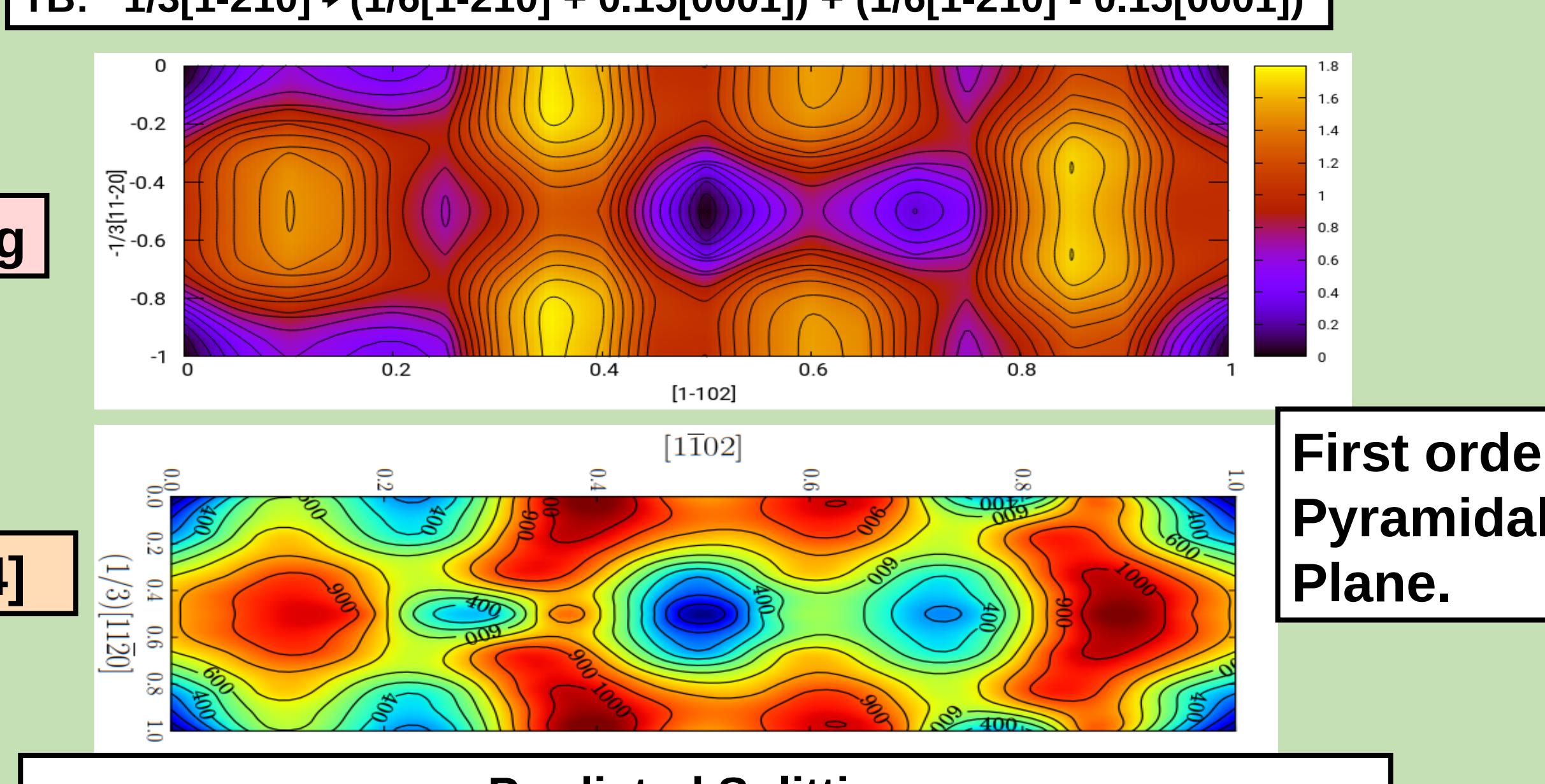
Gamma surfaces are plots of the excess energy of a faulted lattice, compared to an unfaulted one, with respect to fault vector.

- Minima show areas where stable stacking faults occur.
- These predict possible dislocation dissociations in the model.



### Tight Binding

### Pseudopot. [4]



Predicted Splitting:  
Pseudopotential:  $1/3[2-1-13] \rightarrow 4/18[1-102] + 4/18[42-62] + 4/18[2-1-13]$   
TB:  $1/3[2-1-13] \rightarrow 4/18[1-102] + 4/18[42-62] + 4/18[2-1-13]$

## Applications:

- Alloy design.
- Stress-corrosion cracking.
- Electrochemistry.

## References:

- [1] Ghazisaeidi, (2012), Core structure of a screw dislocation in Ti from density functional theory and classical potentials
- [2] Stassis, D. Arch, B. (1979), Lattice Dynamics of hcp Ti.
- [3] Rodney, Ventelon (2016), Ab initio modelling of dislocation core properties in metals and semiconductors
- [4] Ready (2019), Stacking faults and the y-surface on {1-101} pyramidal planes in  $\alpha$ -titanium.