

# **Crystal structure prediction using cluster expansion**

**Kiran Mathew  
5/4/09**

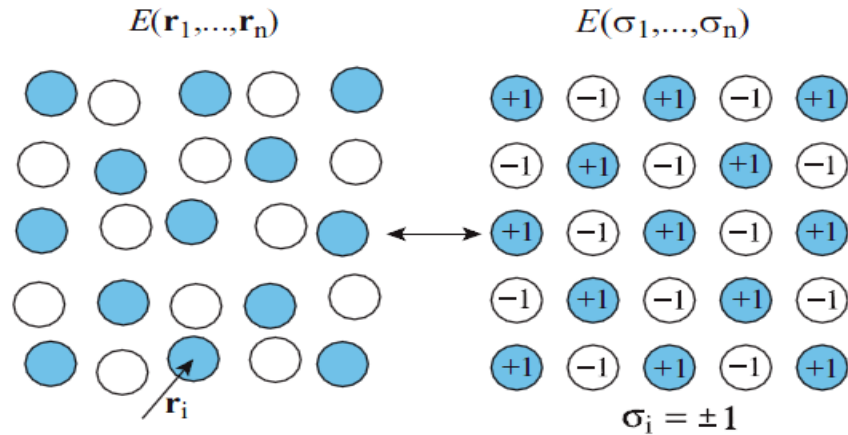
➤ Finding the most **stable crystal structures** of compounds is one of the classical problems in inorganic solid state physics and metallurgy, because knowing the structure of perfect crystalline solids holds the key to material properties

➤ for a **binary  $A_nB_m$**  solid described by a lattice with  $N$  sites, there will be  $2^N$  possible structures

➤ parameterization of the configurational energy so that the dependence of the energy on the configuration can be reproduced with high accuracy-  
**Cluster Expansion**

# The cluster expansion

Alloy system  $\longleftrightarrow$  Lattice model

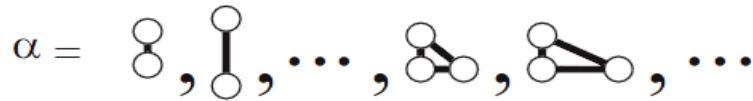


Parametrize configurational-dependence of the energy  $E$  with a polynomial in the occupation variables  $\sigma_i$ :

$$E(\sigma_1, \dots, \sigma_n) = \sum_{\{i,j\}} J_{ij} \sigma_i \sigma_j + \sum_{\{i,j,k\}} J_{ijk} \sigma_i \sigma_j \sigma_k + \dots$$

$$= \sum_{\alpha} J_{\alpha} \sigma_{\alpha}$$

where

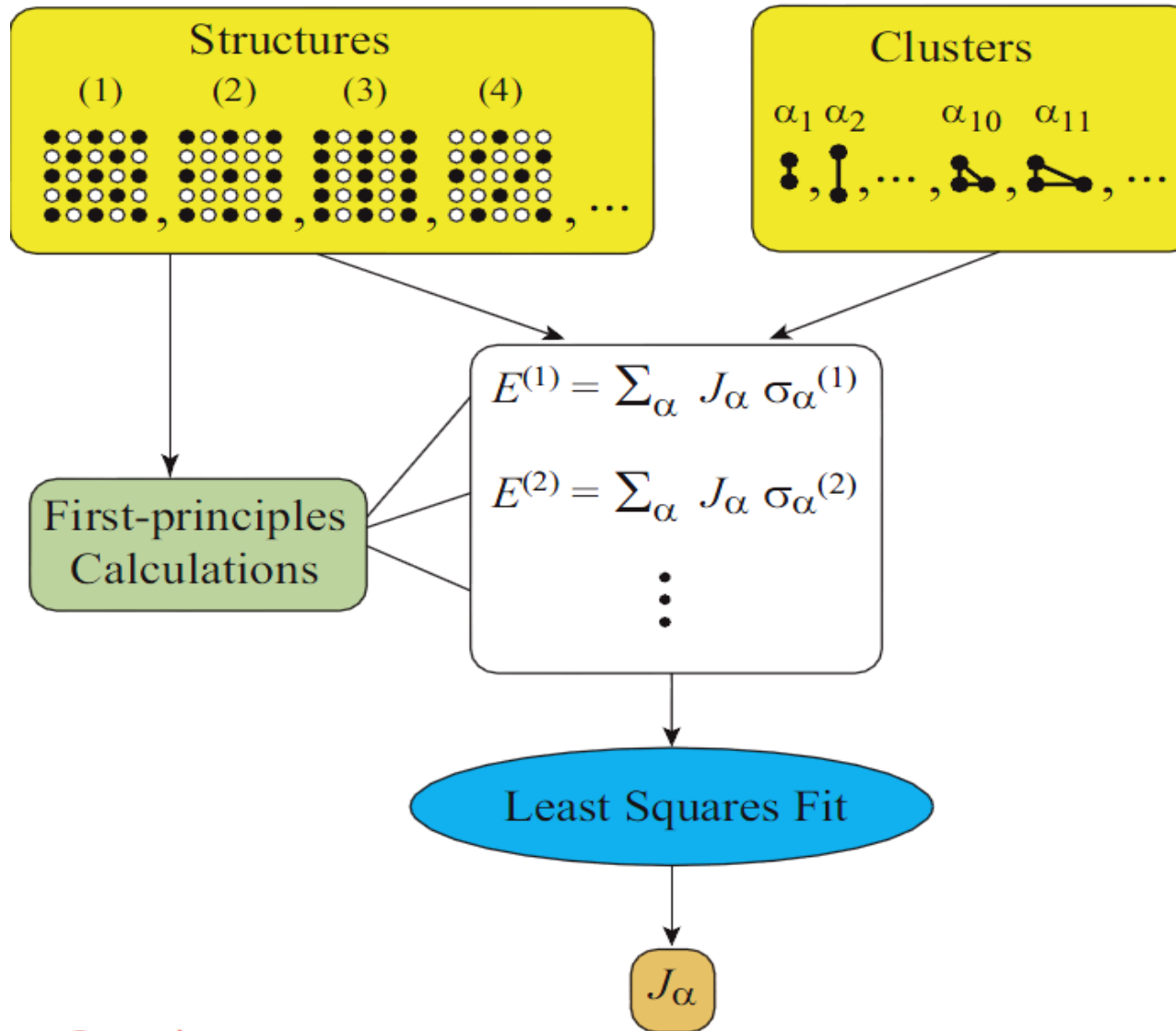


and

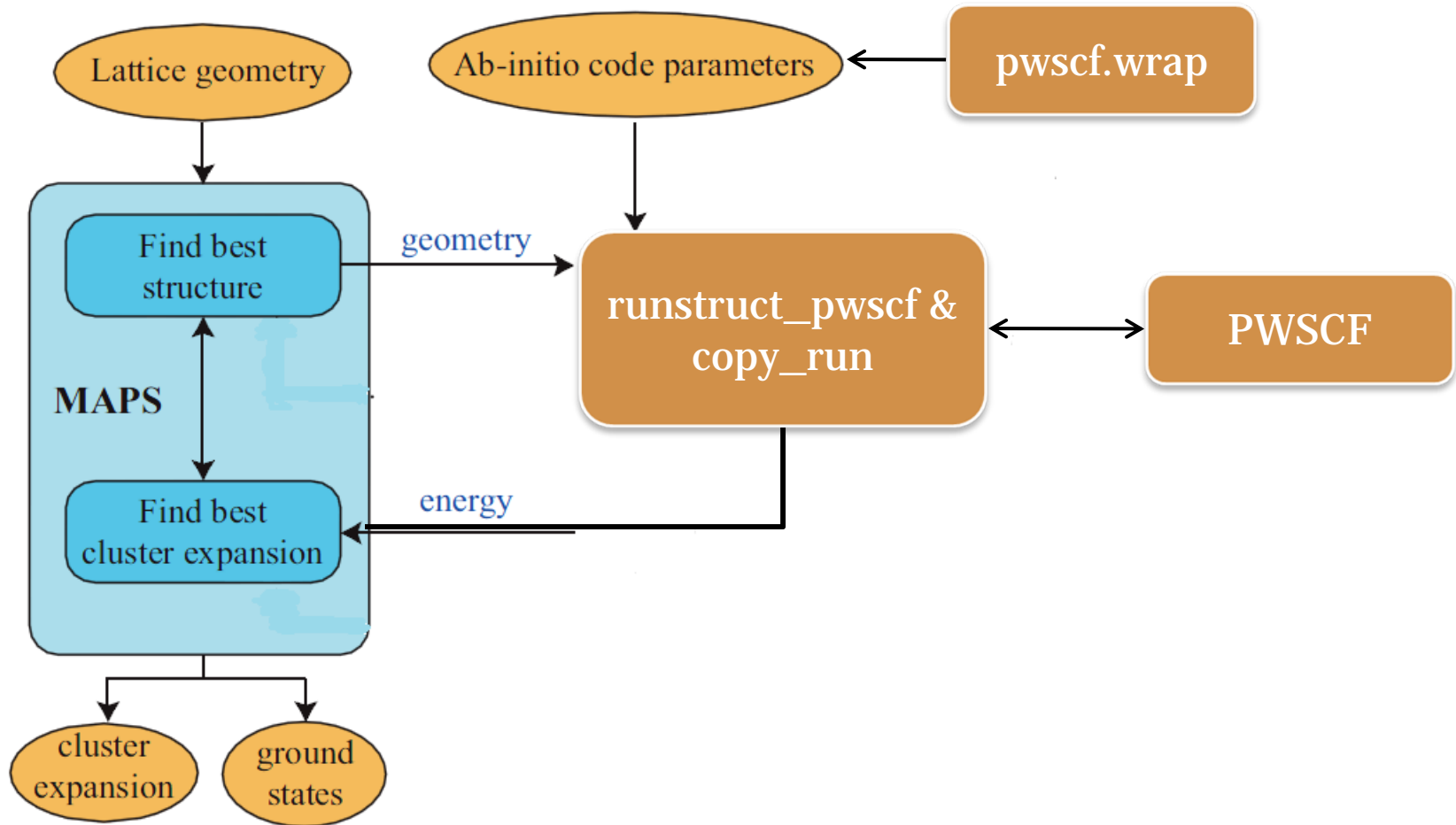
cluster  $\alpha$

$$\sigma_{\alpha} = \prod_{i \in \alpha} \sigma_i = -1$$

# Cluster expansion fit



# Cluster expansion construction module (MAPS)



# Examples

➤ Two systems considered

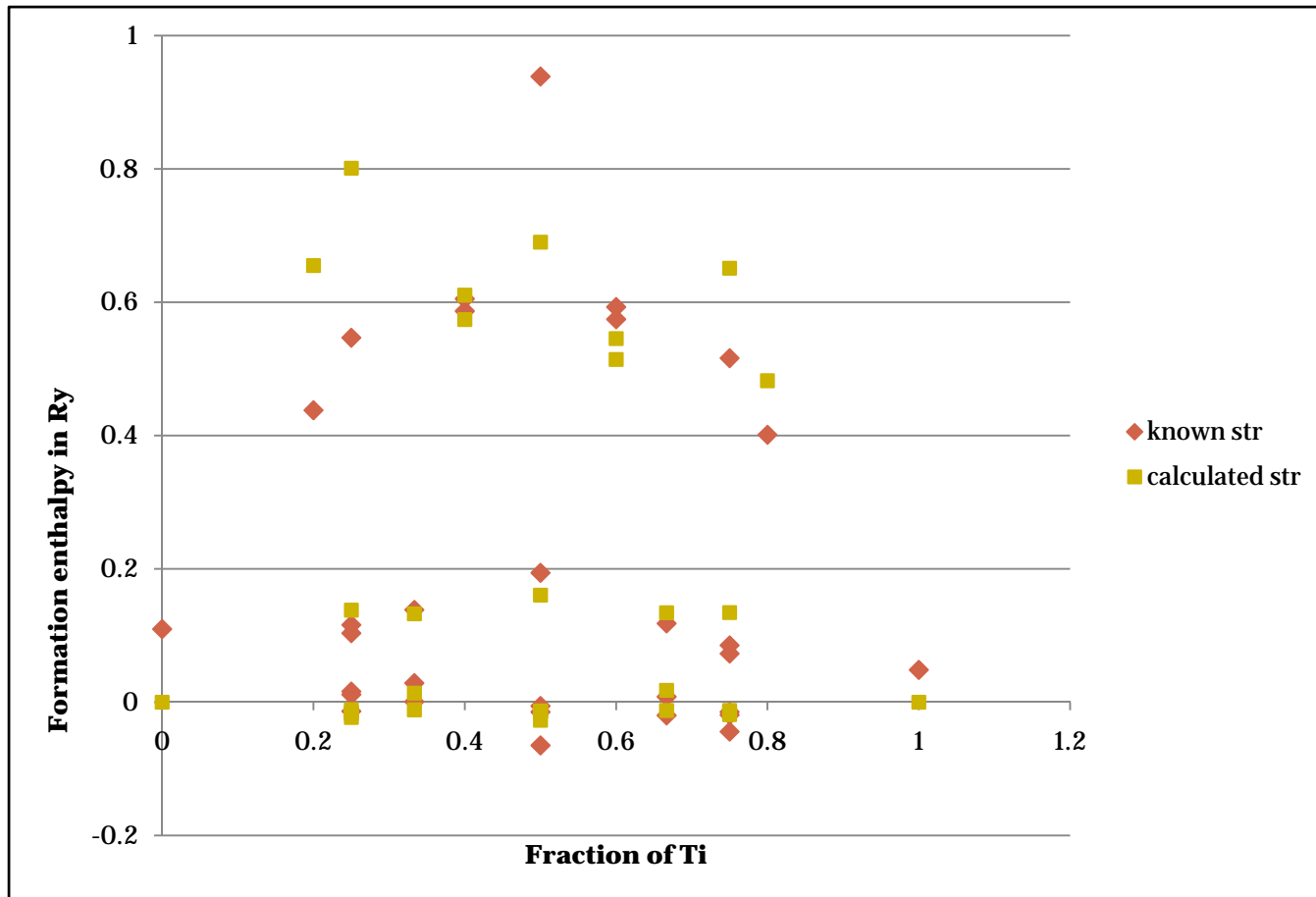
FCC Al-Ti

HCP Al-Ti

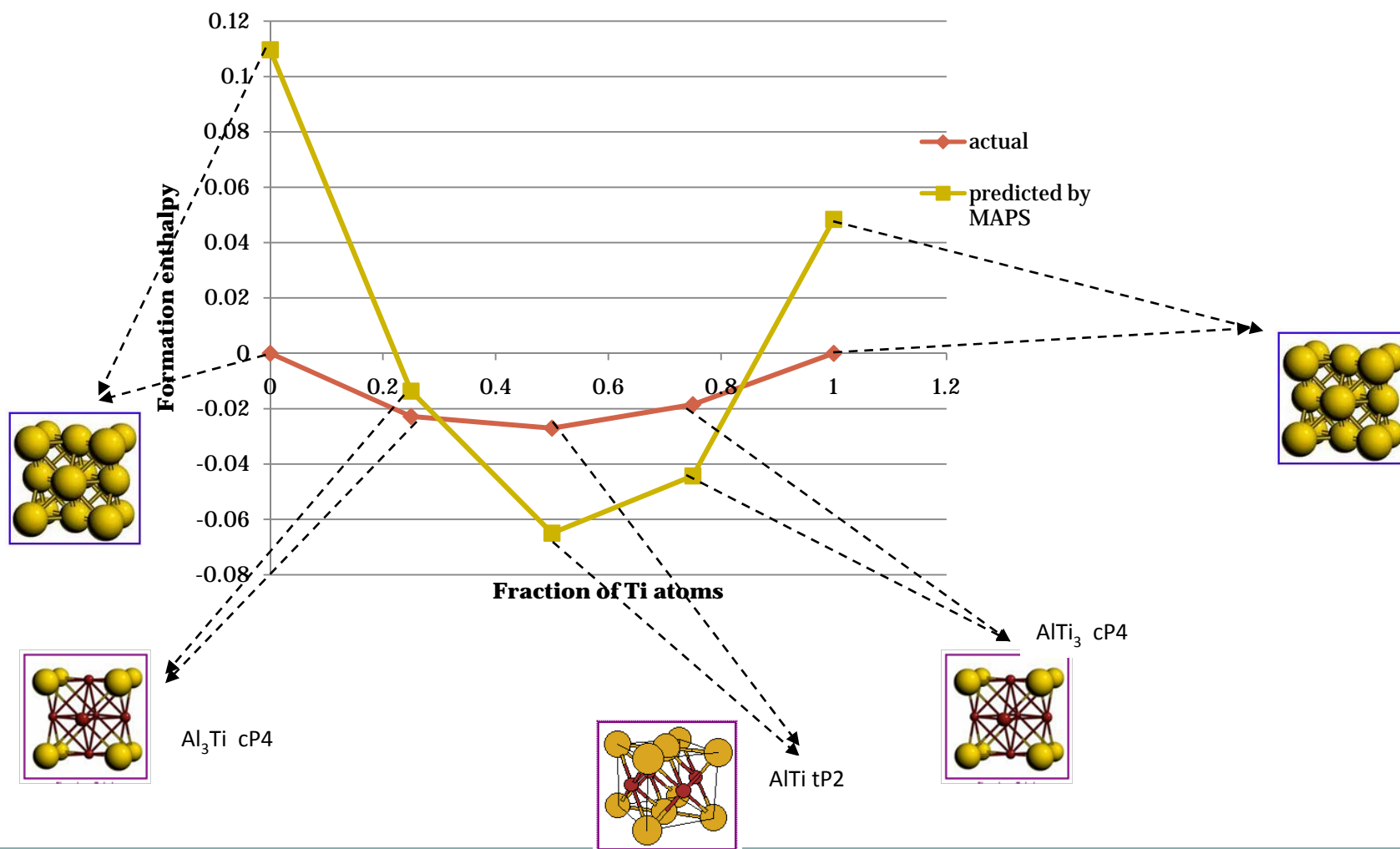
➤ 40 structures used for learning the cluster expansion

➤ Computationally demanding: required 2-3 days for the calculation of the energies of 40 structures and the corresponding cluster expansion.

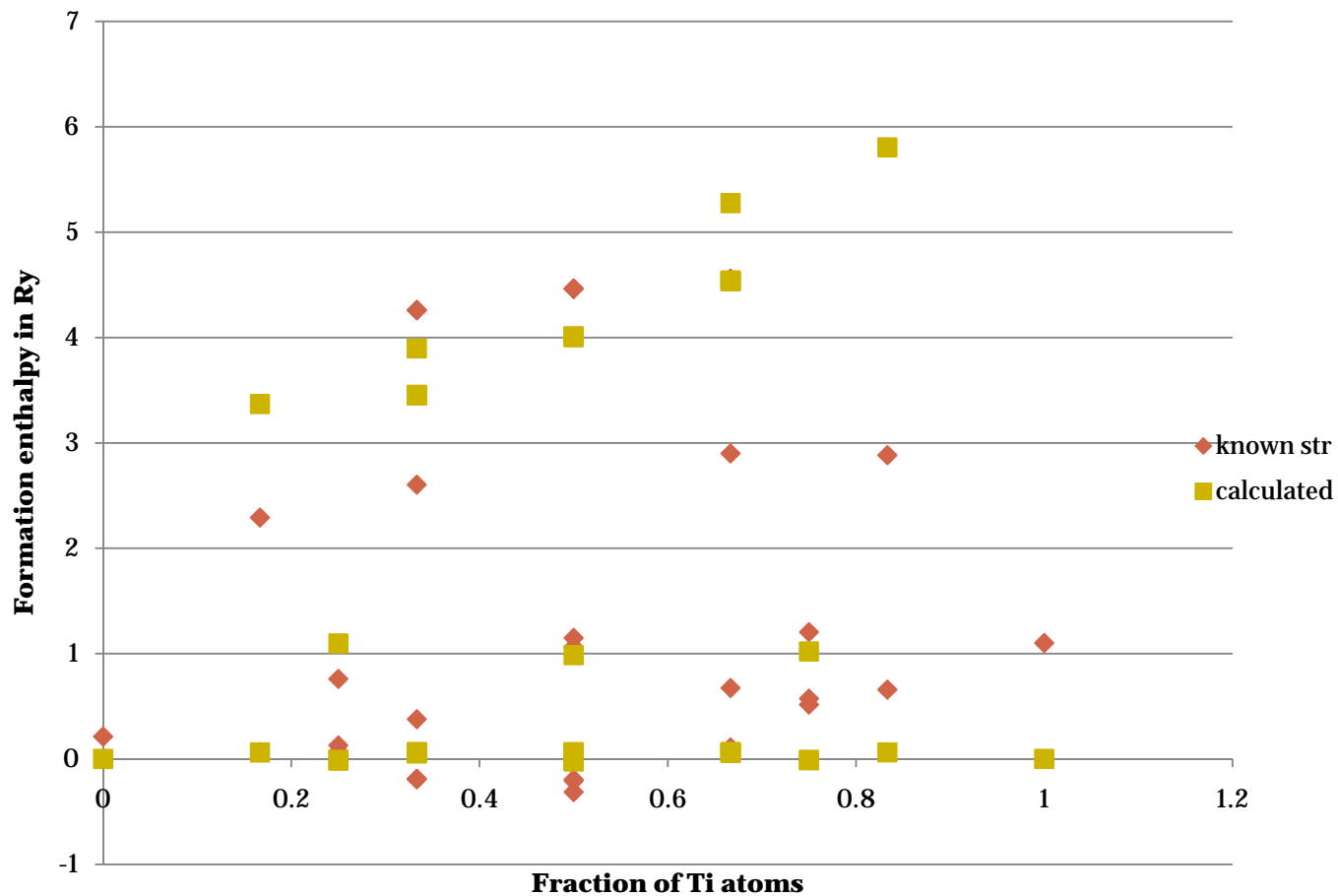
# 1. FCC Al-Ti system



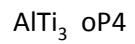
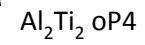
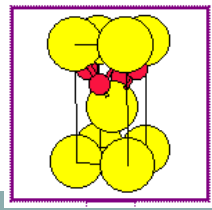
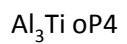
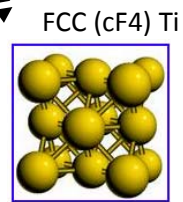
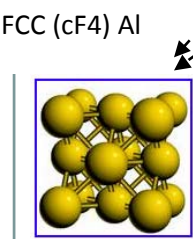
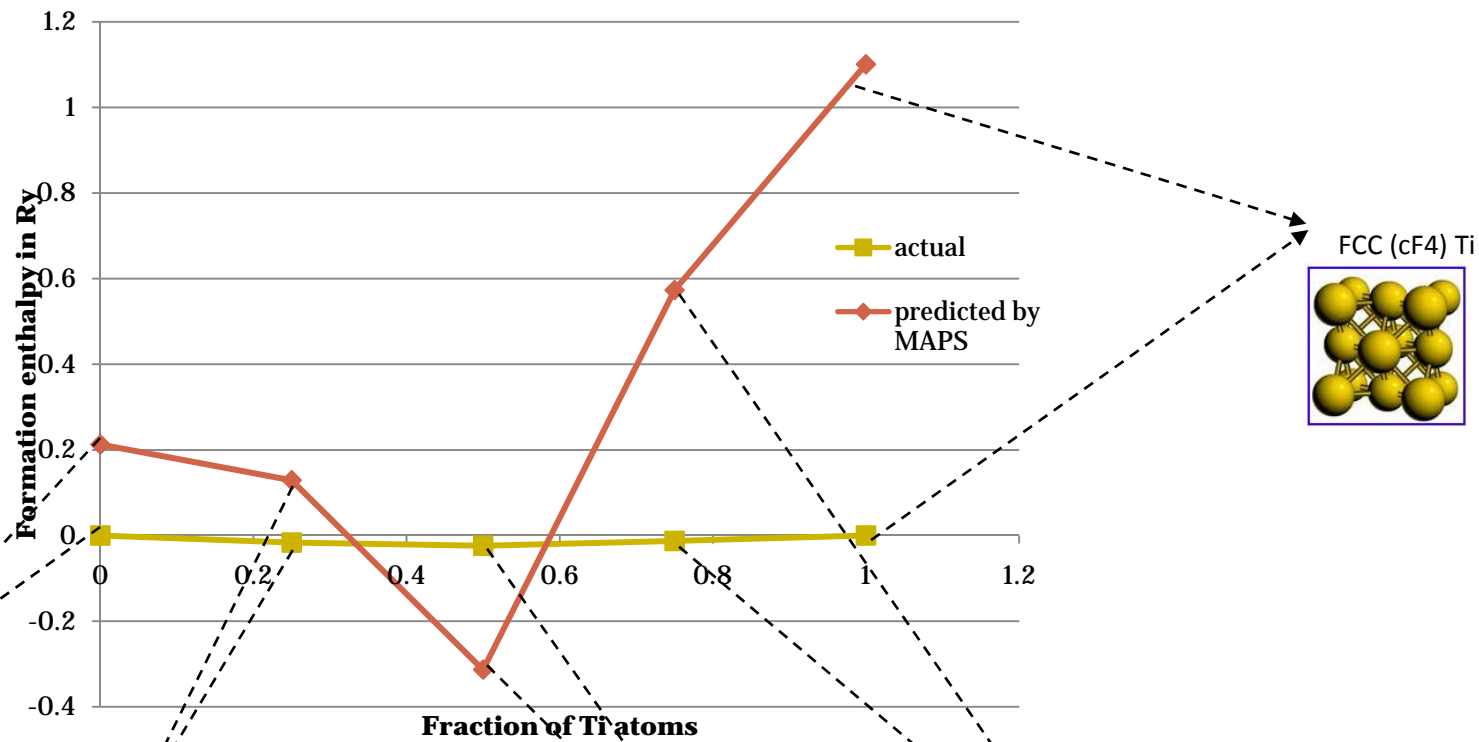
# Ground States



## 2. HCP Al-Ti system



# Ground States



# Conclusions

- Reasonable cluster expansion for FCC Al-Ti
- Error too high for the HCP system!!
- Input structure requirements vary from structure to structure  $\Rightarrow$  certain structures could be computationally expensive.
- Main limitation : can be applied only to a fixed parent lattice structure, but several other phases are known to exist