Ab initio and KMC study of ODS solute interactions with point defects in Fe-Cr alloys

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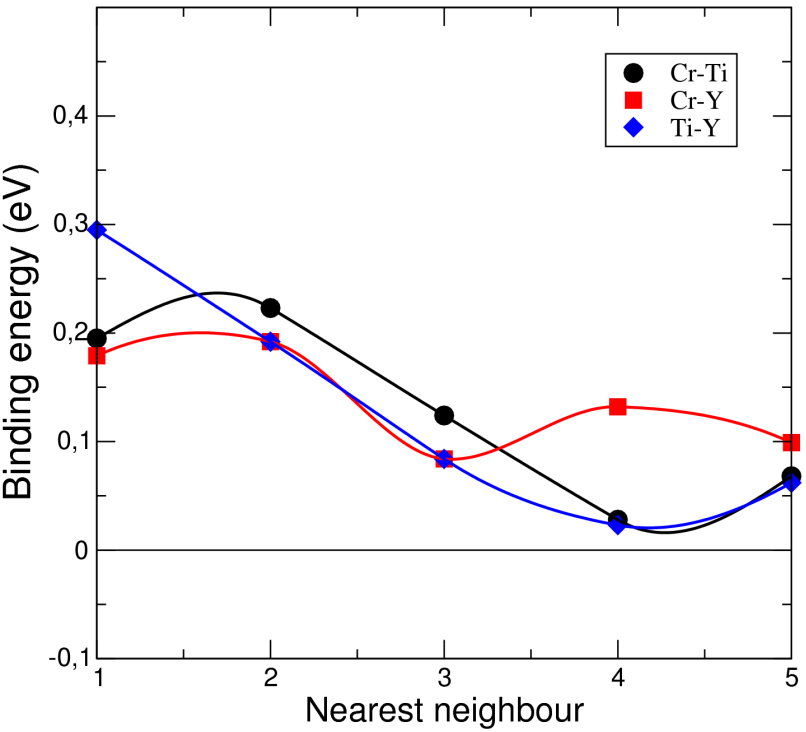
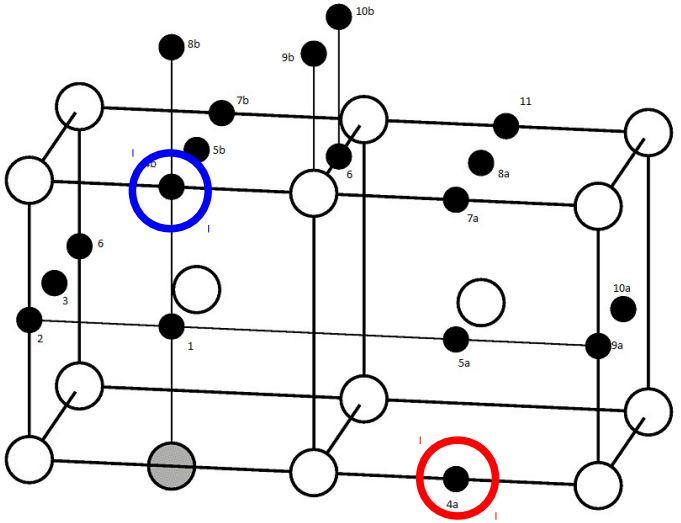
Most of the results in:
Claisse and Olsson, NIMB 303 (2013) 18–22

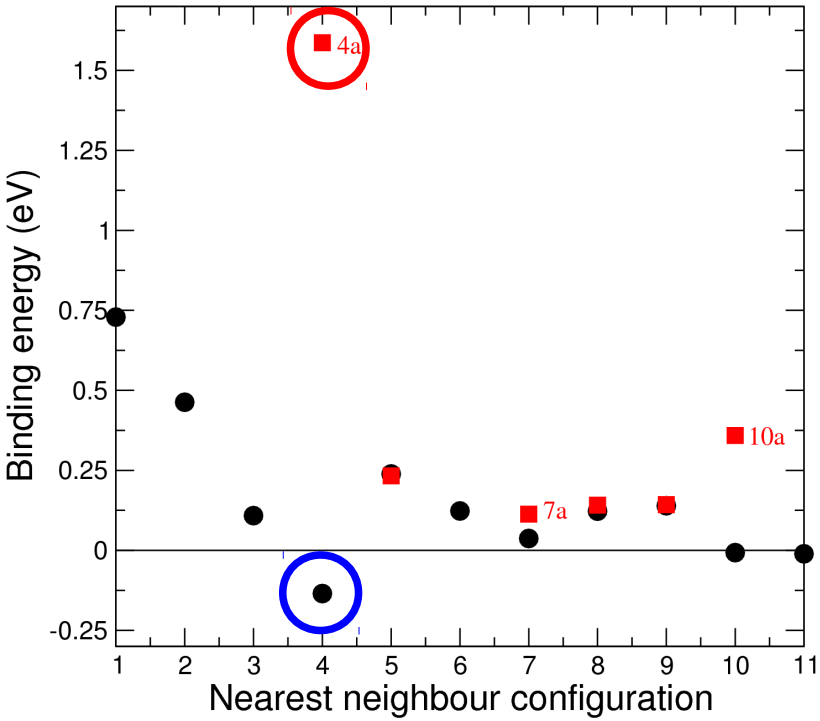
Solute – solute interaction in bcc Fe

- All substitutional solutes repel each other
- Oxygen binds Cr (1nn), Ti (1,2nn), Y (2nn)
- Oxygen binds oxygen at 4nn distance (in 4/6 4nn sites)



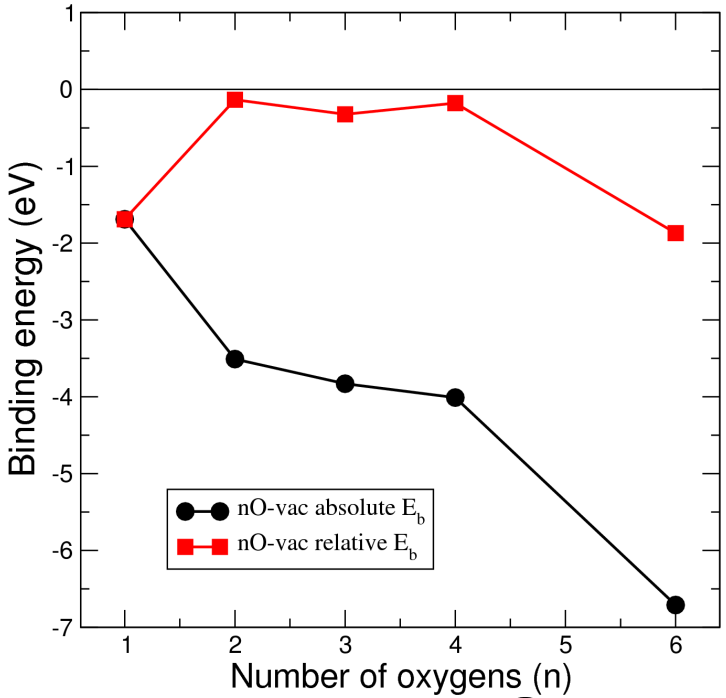
config	Binding energy (eV)
Y-O 1nn	0.32
Y-O 2nn	-0.73
Ti-O 1nn	-0.23
Ti-O 2nn	-0.46
Cr-O 1nn	-0.10
Cr-O 2nn	0.06





Solute – vacancy interaction in bcc Fe

- Vacancies bind oxygen strongly
- Binding decreasing with distance
- Up to 6 oxygen can bind to one vacancy!



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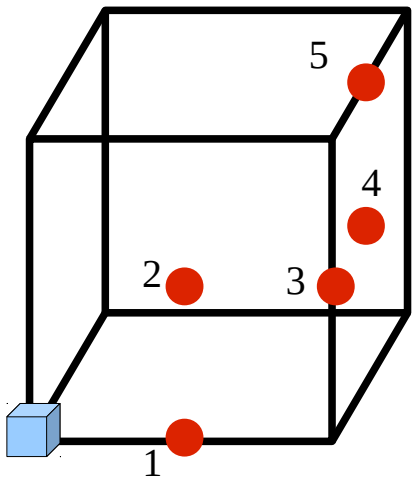
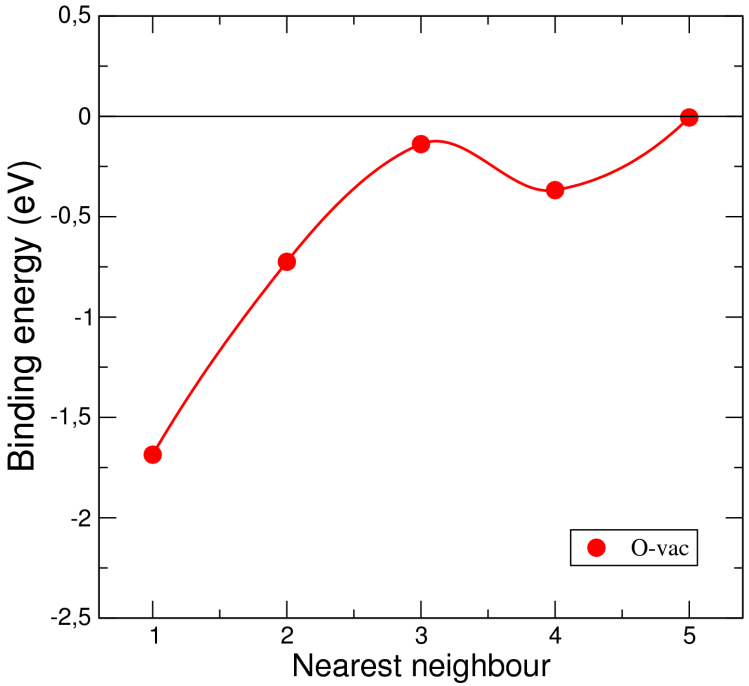
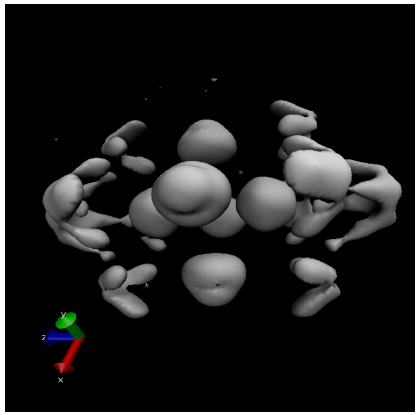
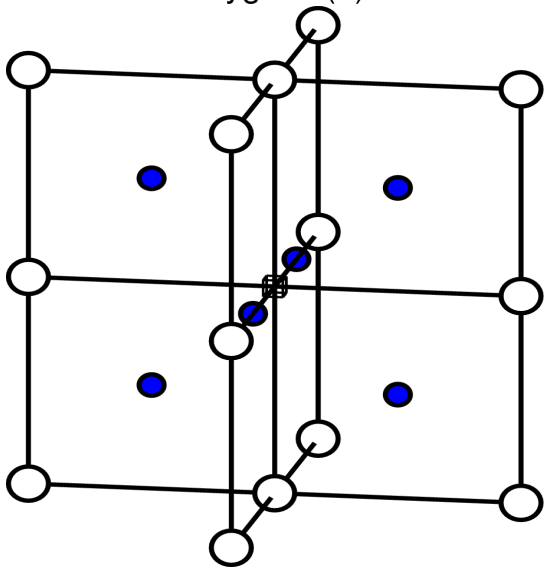
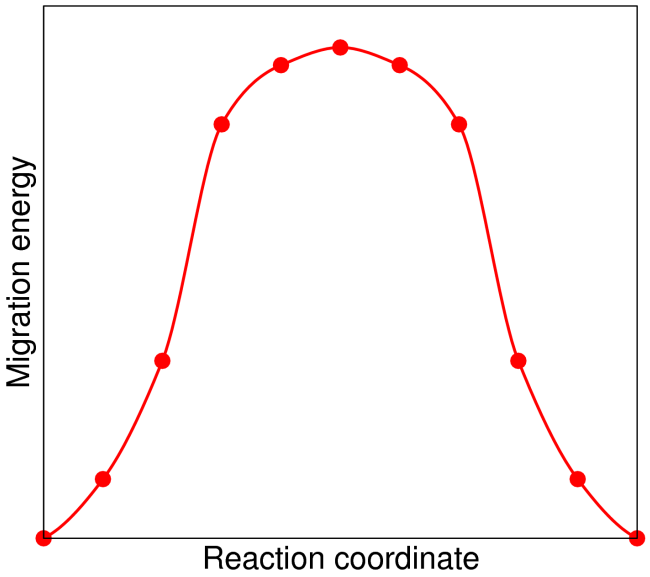


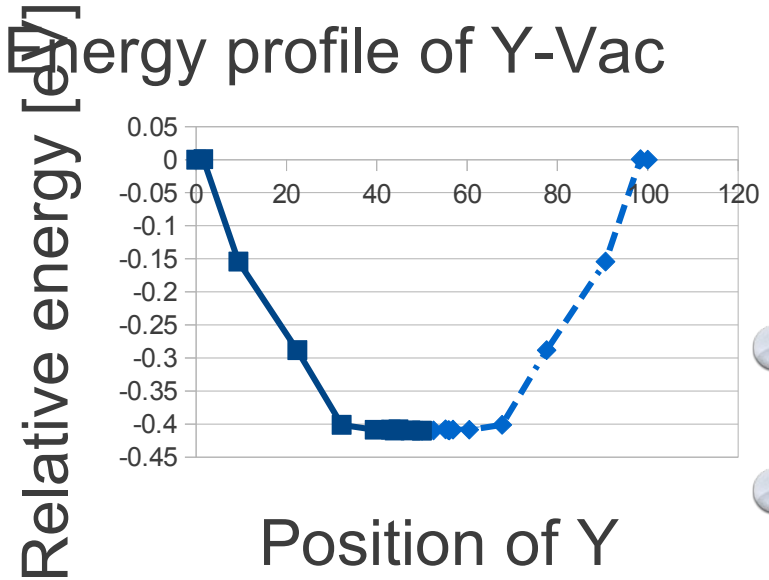






Solute migration barriers in bcc Fe

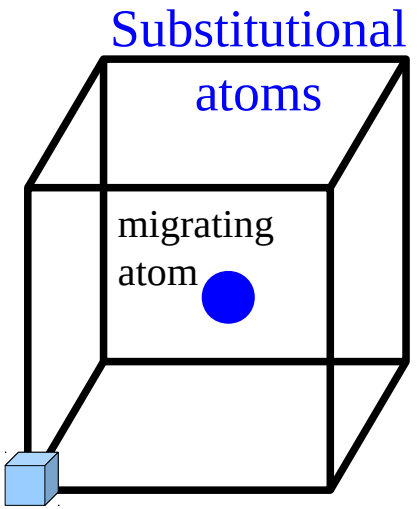


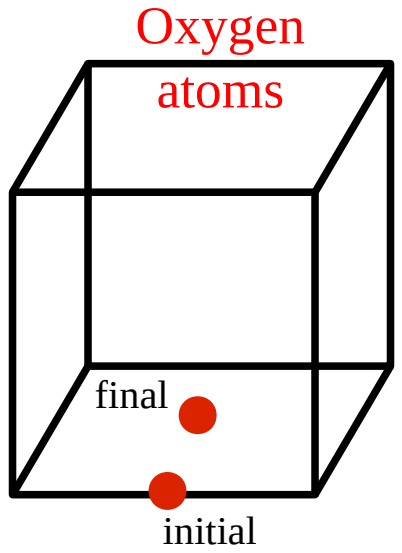


- The migration barriers of the different solutes have been calculated using the climbing image NEB with 3 images

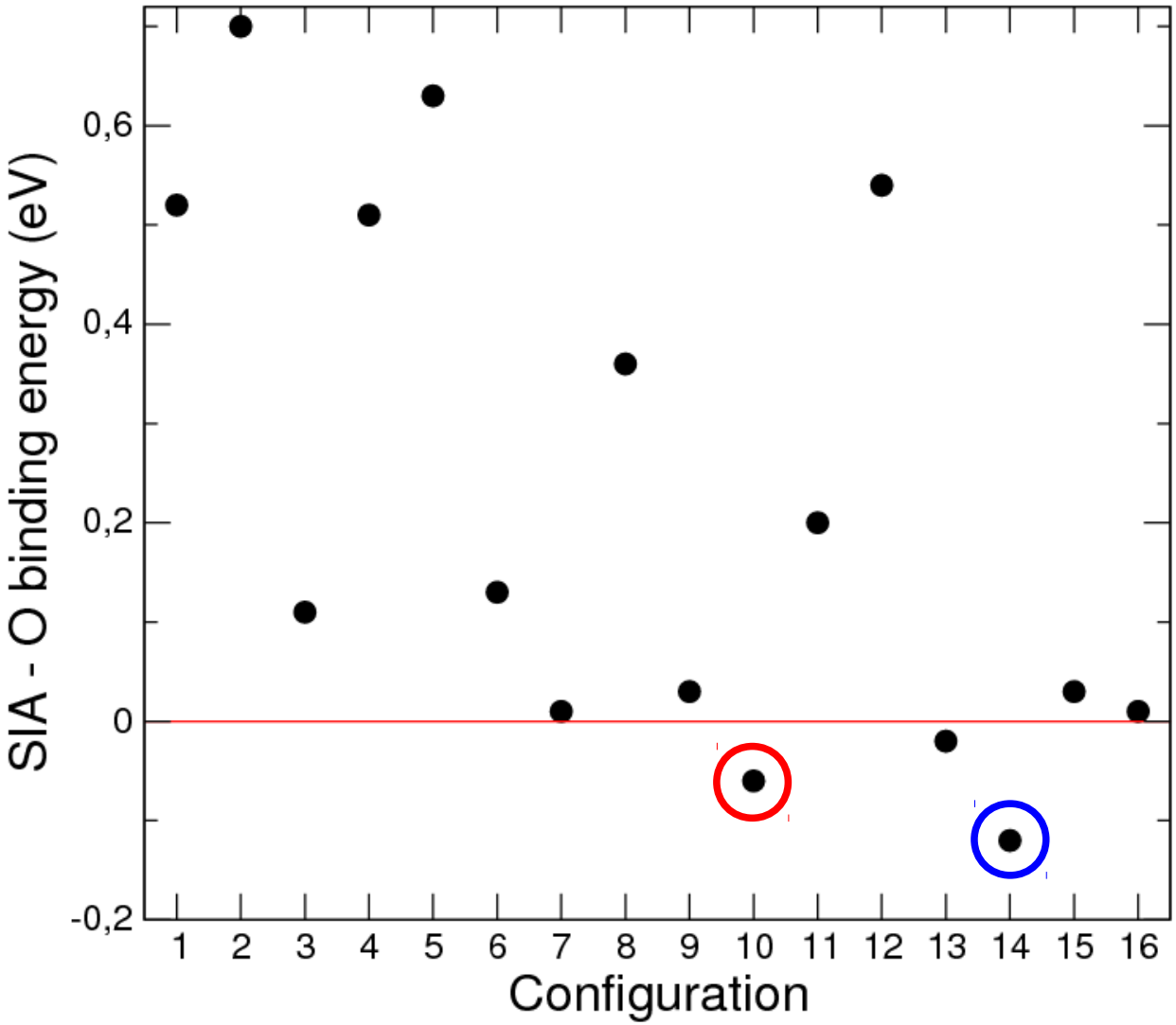
Solute atom	Migration energy (eV)
Fe (host)	0.71
Cr	0.54
Ti	0.38
Y	*
O	0.48

- Y special case: Its relaxed position is at the saddle point
- No single vacancy mitigated Y migration!

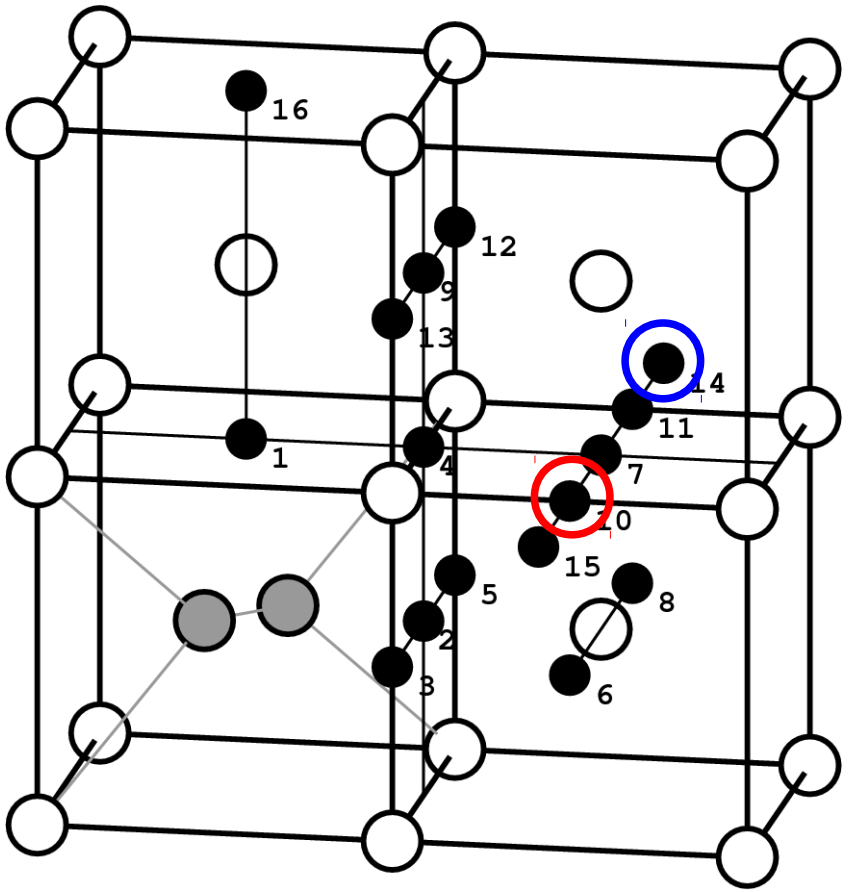




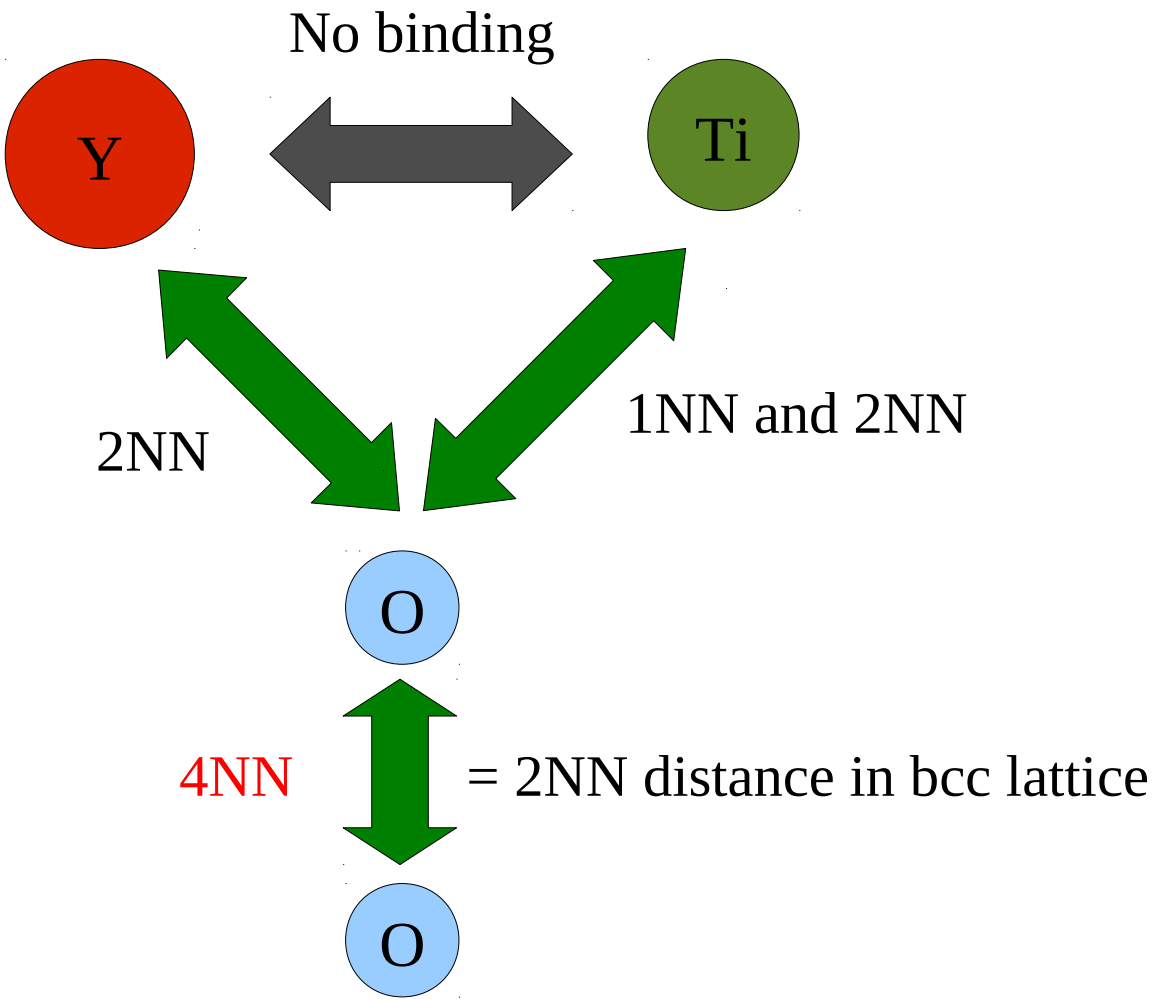
Oxygen – self-interstitial interaction



- Oxygen – SIA interaction is repulsive at close range
- Exhibits long range interaction
- Mixed Cr-SIA same as pure Fe



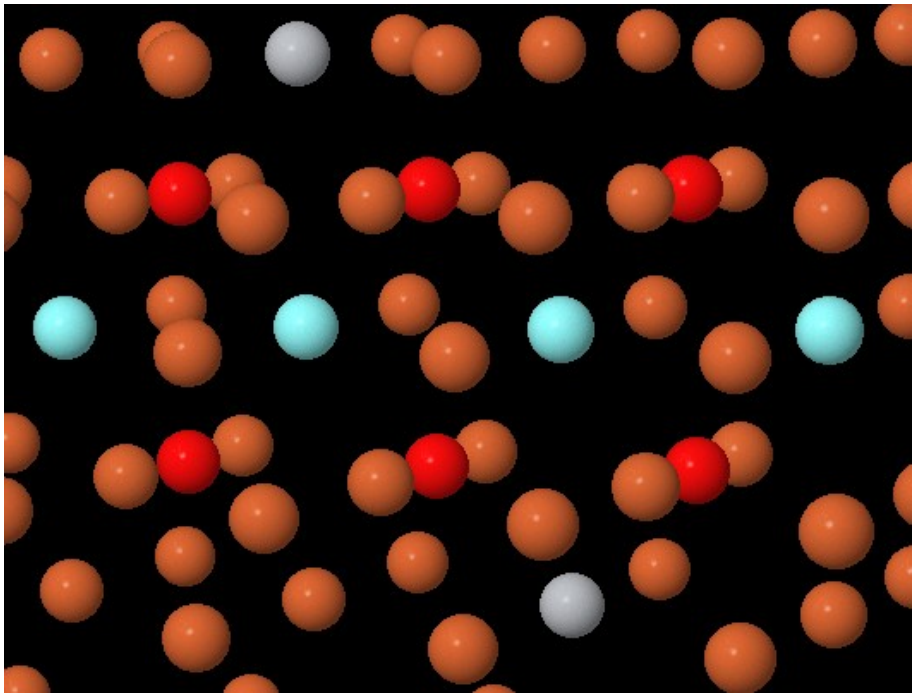
ODS solute binding summary

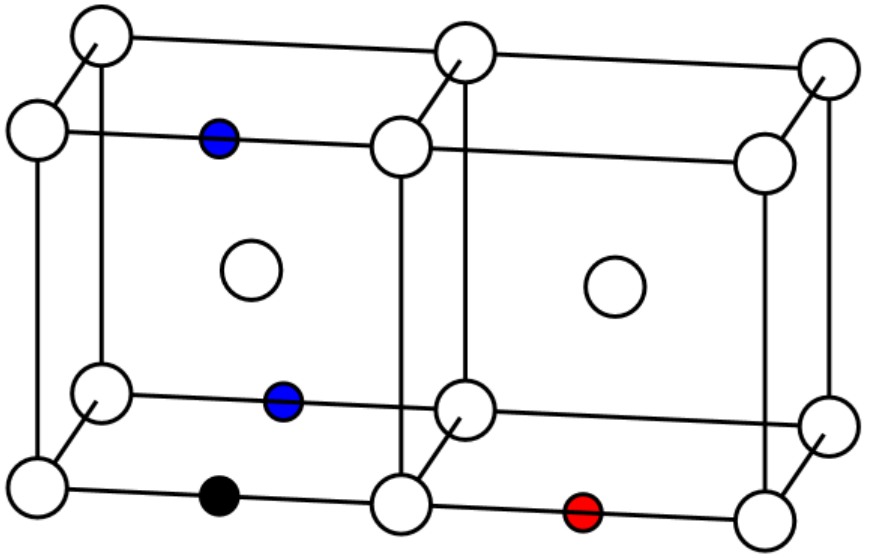


+ vacancies binding with these 3 solutes
+ SIA binding with Cr (and Y,Ti,O in less important configs)

ODS cluster nuclei

- According to these pair interactions, we can expect the most stable ODS cluster nuclei to have Y and O in the center, and Ti decorating the edge





- Due to the oxygen-oxygen preferential directionality (4nn, no Fe in between) **this inescapably leads to planar structures!**
- Vacancies (or very strong structure relaxation) are needed in order to break the 2D preference

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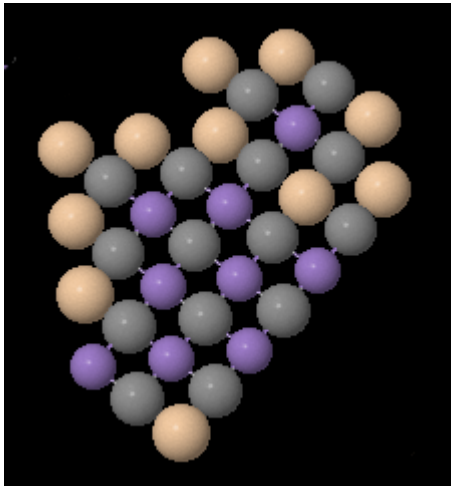
KMC simulations

KMC simulation of cluster formation at 600K using the DFT based current parameterization

Planar clusters form

O-Y in center
Ti on edge



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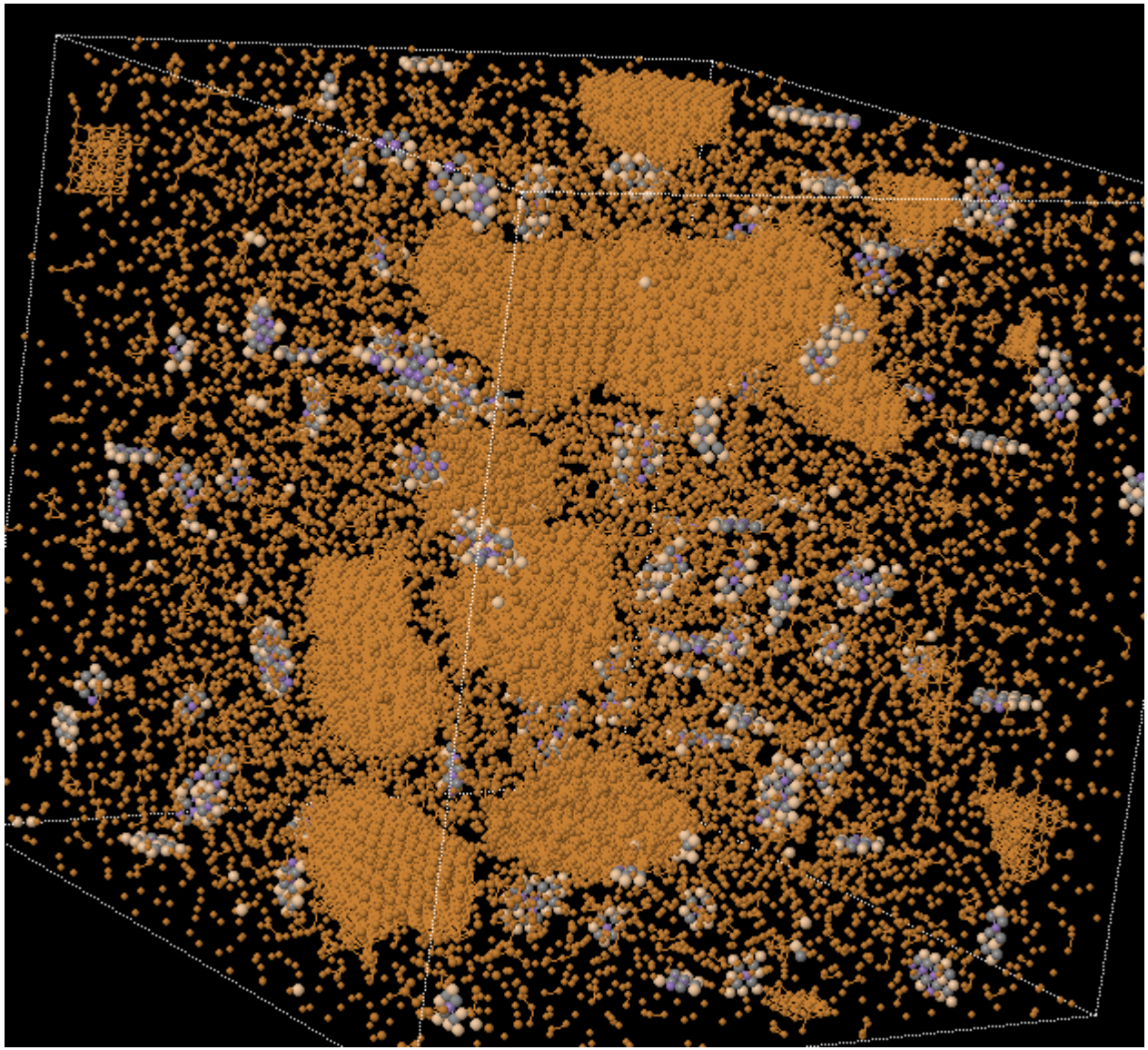
Metropolis MC simulation – the role of Cr



- The presence of Cr seems not to strongly affect the cluster stability
- If in Cr segregated state, the ODS clusters form in the α-phase

Conclusions

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- The behavior of Yttrium diverges from the general transition metal trend
- Single vacancies can be very efficient oxygen traps
- The oxygen-oxygen interactions control the cluster geometry
- Yttria nucleation on vacancies very likely – but planar nuclei very stable even without vacancies
- Nucleation of oxide clusters in planar form according to DFT and KMC model
- Vacancies and crystal distortion will allow for spherical growth

Outlook

- To adjust the model to allow for formation of stable 3D clusters
- To perform systematic long time simulations of the formation stages at different temperatures
- To characterize the nucleation stage and better identify the mechanisms of formation (and re-formation)
- To simulate the behavior of small clusters under neutron irradiation conditions

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