

# Structure determination of YbCd icosahedral quasicrystal

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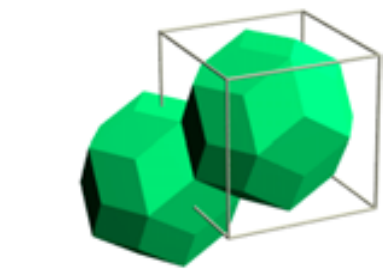
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# Outline

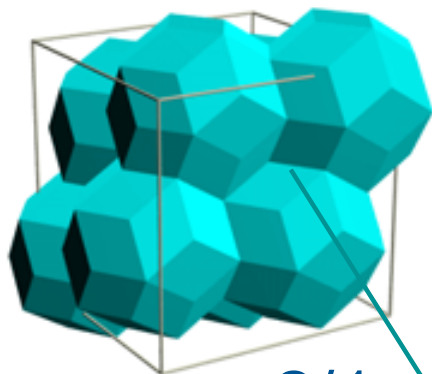
- Building units and their connection scheme in approximant crystals
- Ideal structure of Yb-Cd i-QC
- Cluster arrangement in Yb-Cd i-QC
- 6D structure and 3D structure
- Refined structure model of Yb-Cd i-QC
- Summary

# Building units and their connection scheme in approximant crystals

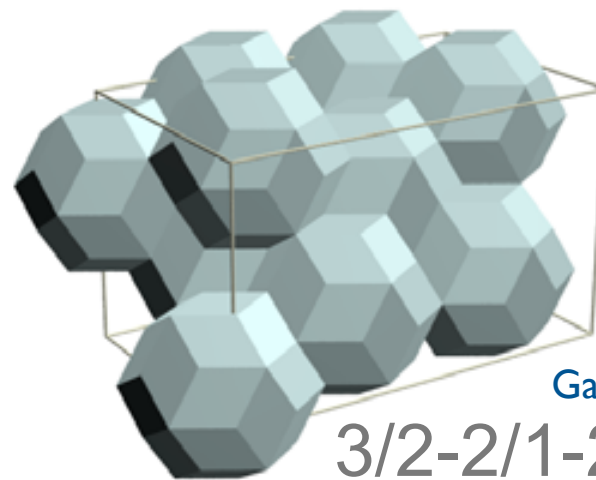
# Various approximant crystals



Many examples  $1/1$

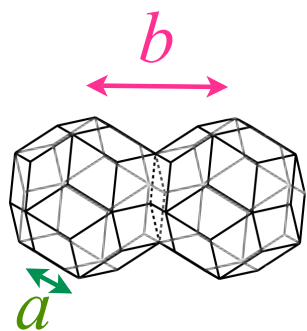


Al-Mg-Zn  
Cd-Ca etc.  $2/1$

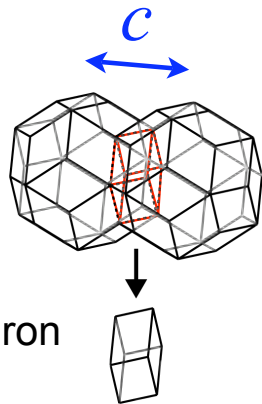


Ga-Mg-Zn  
 $3/2-2/1-2/1$

Linkages



rhombic triacontahedron (RT)

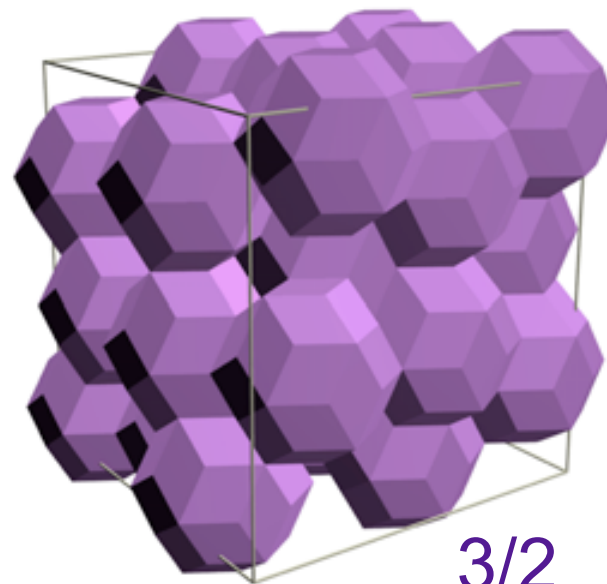


obtuse rhombohedron (OR)

acute rhombohedron (AR)

$$b \equiv (4 + 8/\sqrt{5})^{1/2} a$$

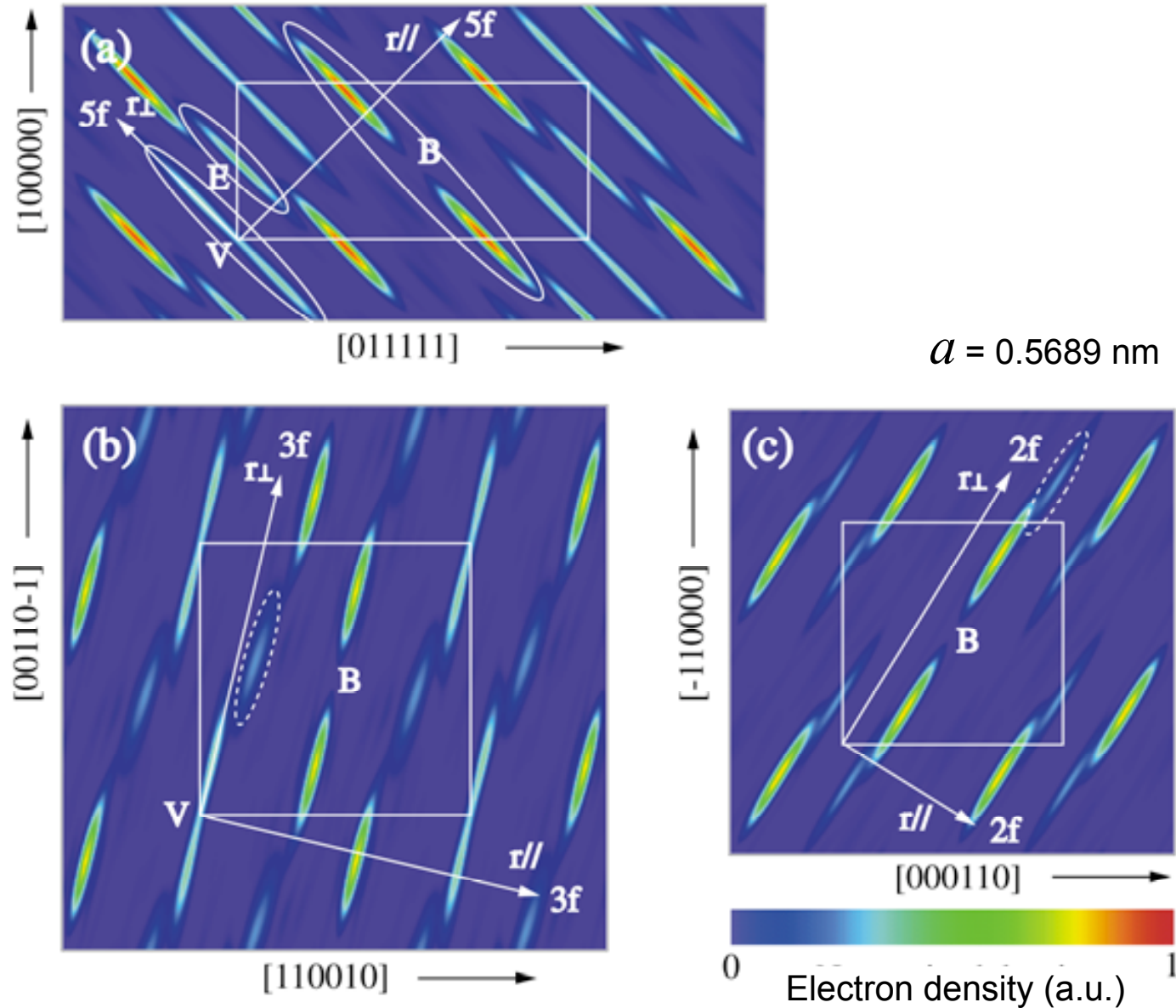
$$c \equiv (\sqrt{3}/2) b$$



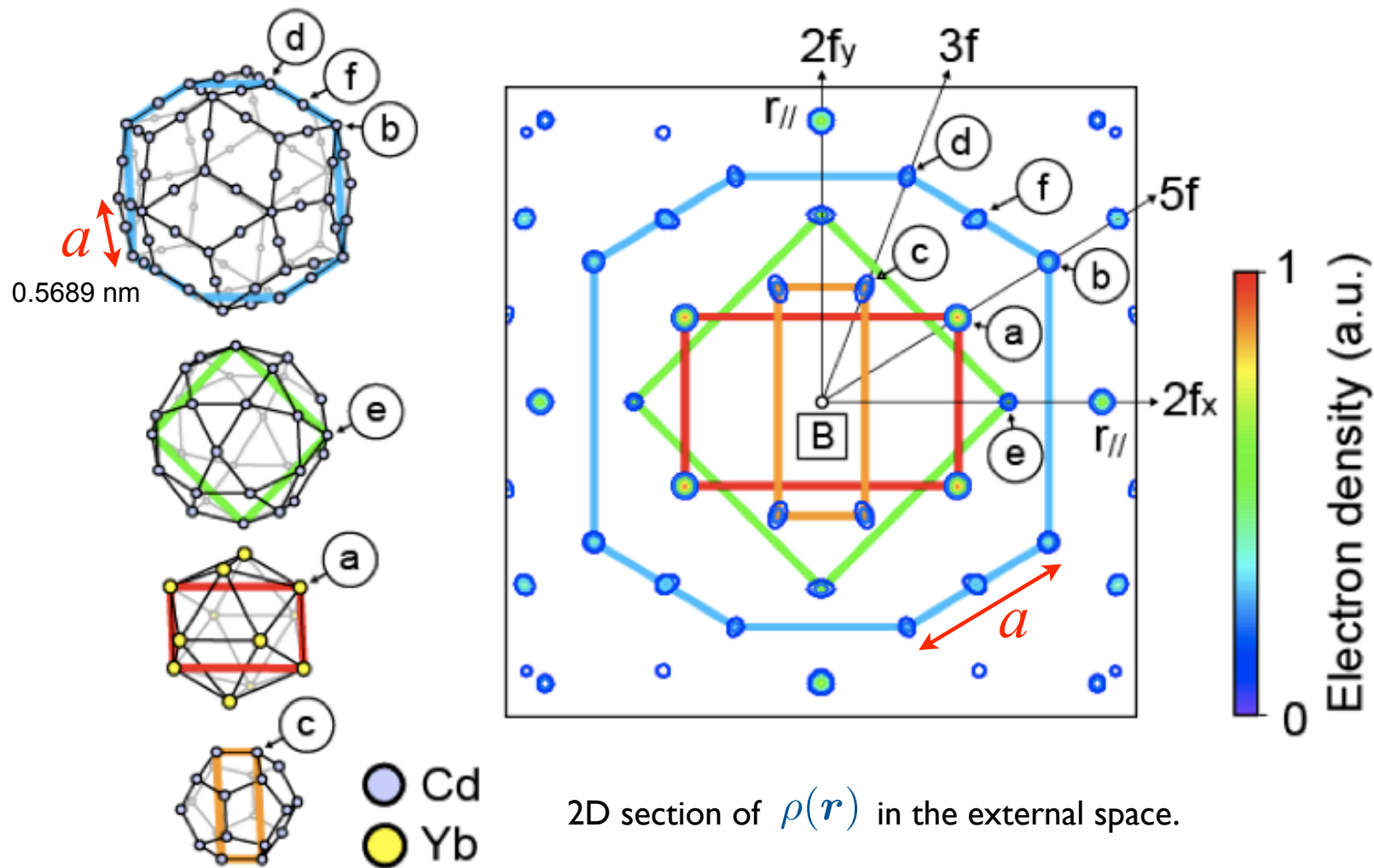
$3/2$

RT cluster in Yb-Cd i-QC's  
and  
its atomic decoration

# Reconstructed 6D electron densities of i-YbCd<sub>5.7</sub>

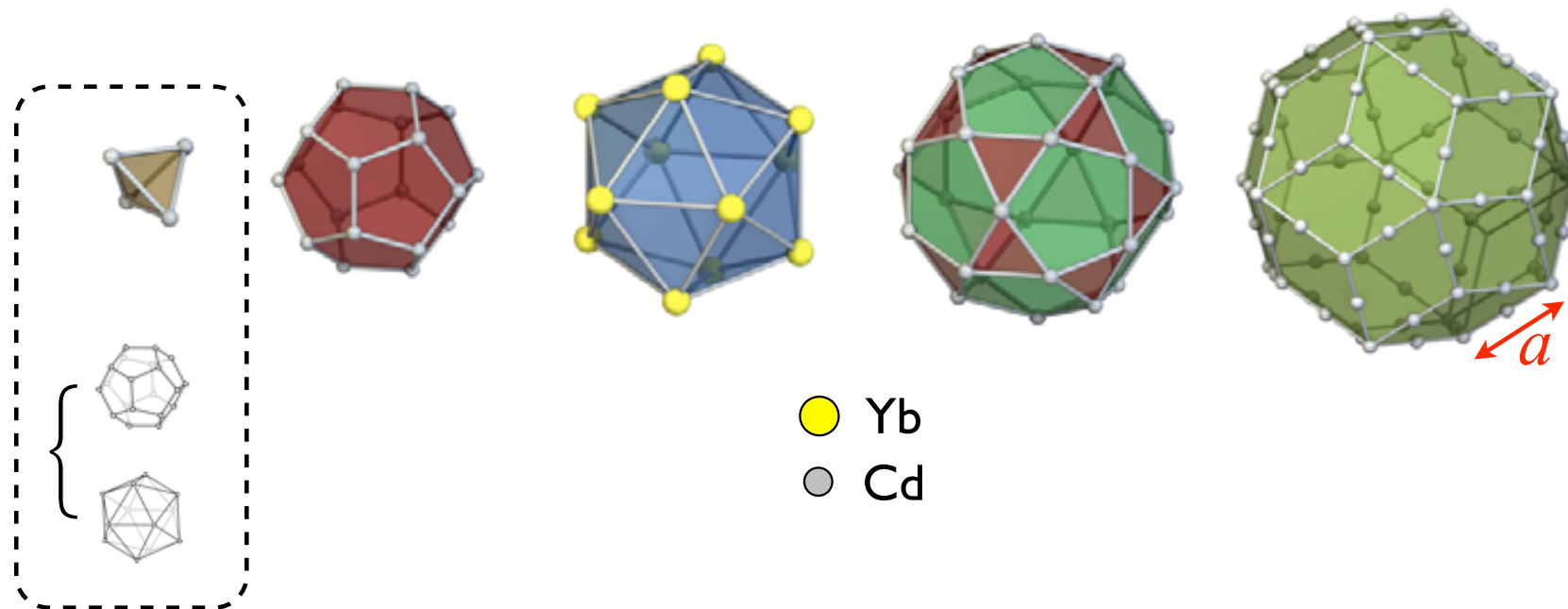


# Interpretation of the reconstructed densities



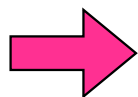


# Idealized RT cluster in Yb-Cd i-QC



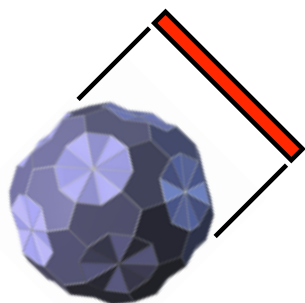
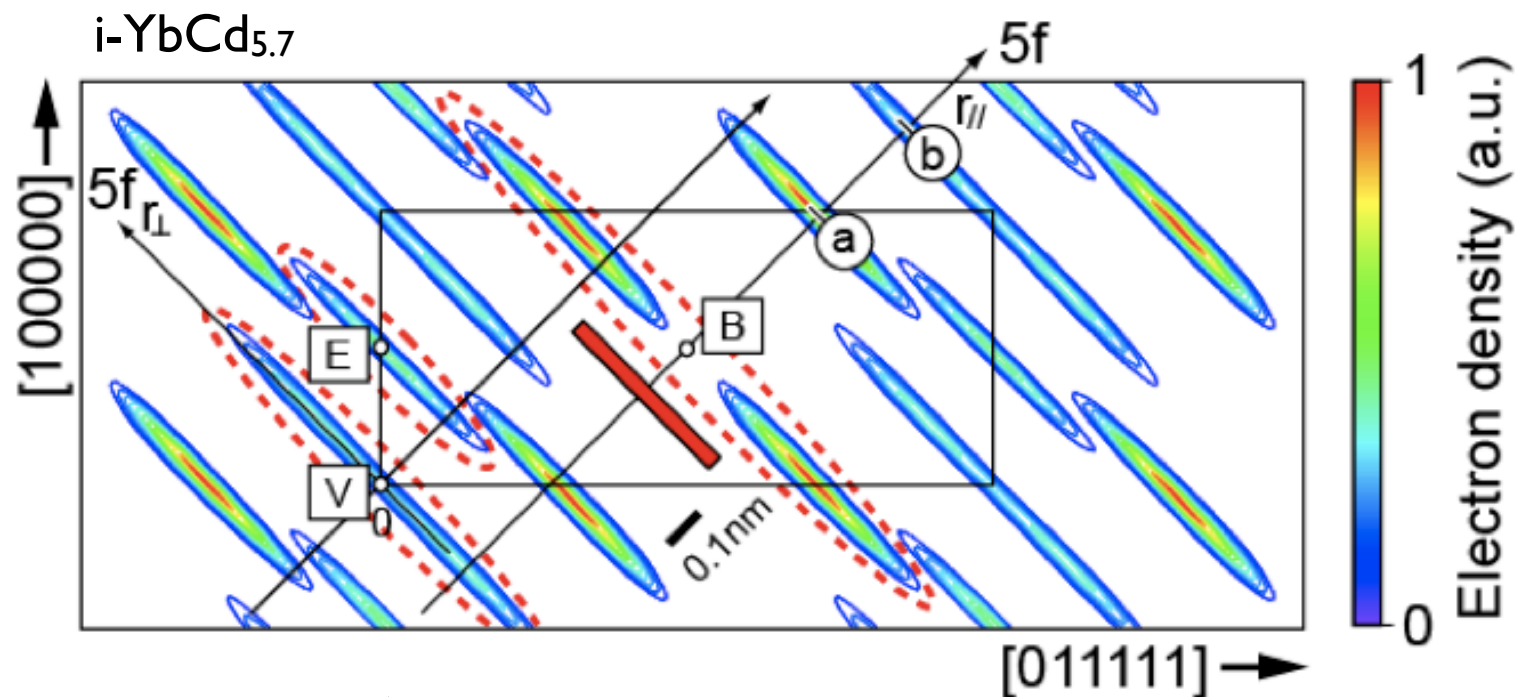
## Model construction of YbCd i-QC

- RT, AR, and OR as building units.
- $b$ - and  $c$ -links for RT units.
- RT unit has an edge length of  $a$ .



12-fold vertices of 3DPT with an edge length of  $a$  as the positions of the RT's.

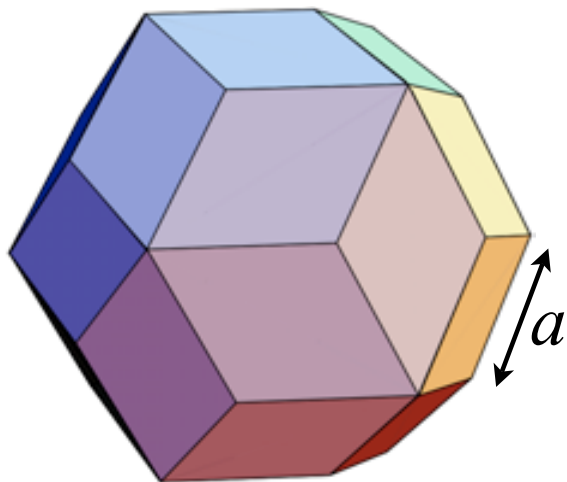
# Evaluation of the size of occupation domain for the cluster centers



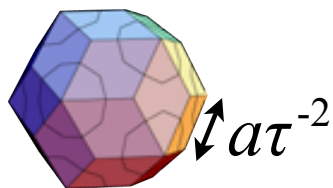
Size of the hole fits occupation domain for the 12-fold vertices of 3DPT with an edge length  $a$

# Occupation domains

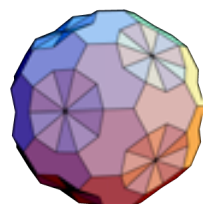
What generates these OD's ?



Vertices of the **3DPT**  
with edge length  $a$

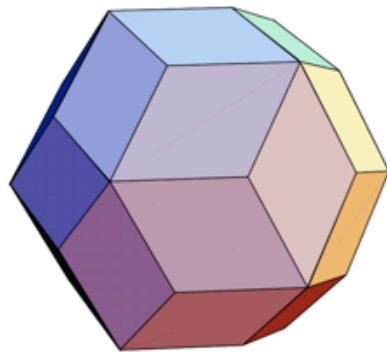


12-fold vertices

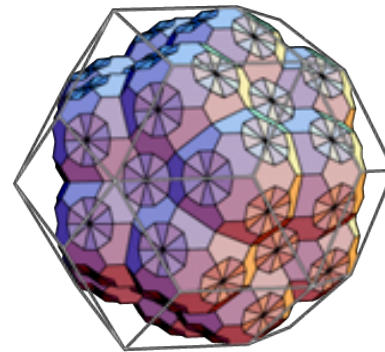


12-fold vertices with  
only  $b$ - and  $c$ -links

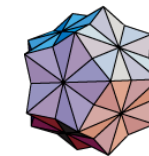
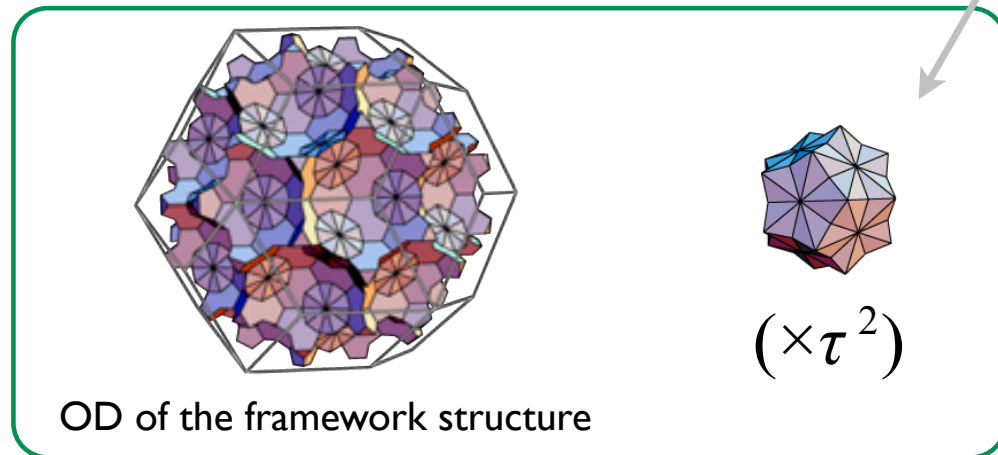
# The occupation domain of the framework structure



3DPT

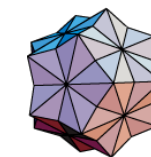


RT's at 12-fold vertices of the 3DPT



$(\times \tau^2)$

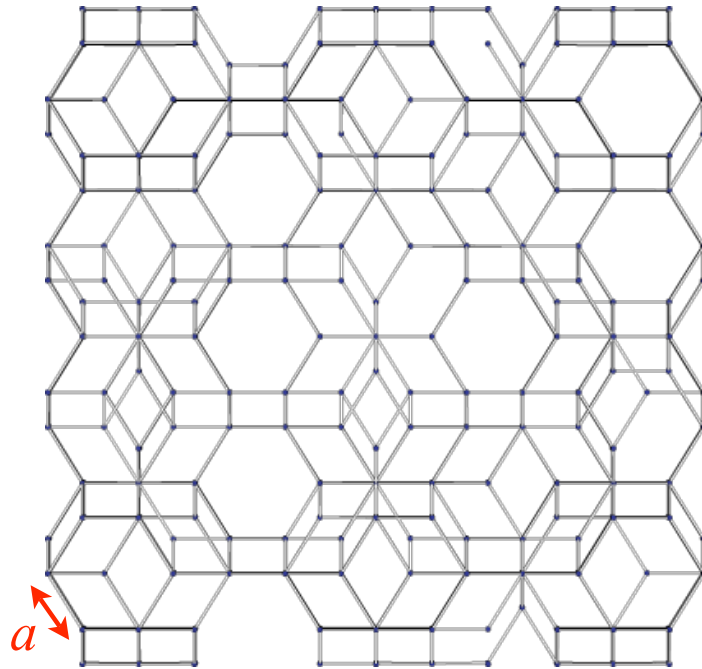
shape of hole  
at the center



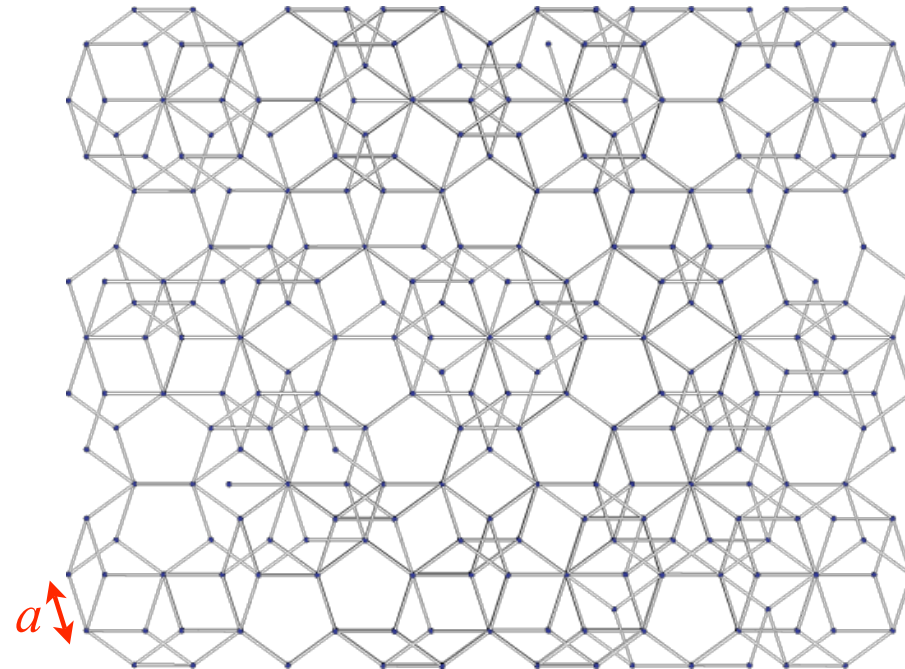
$(\times \tau^2)$

# Framework structure of Yb-Cd i-QC model

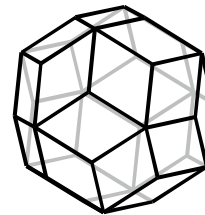
2-fold projection



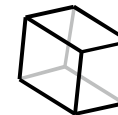
5-fold projection



Three building blocks:



**RT**



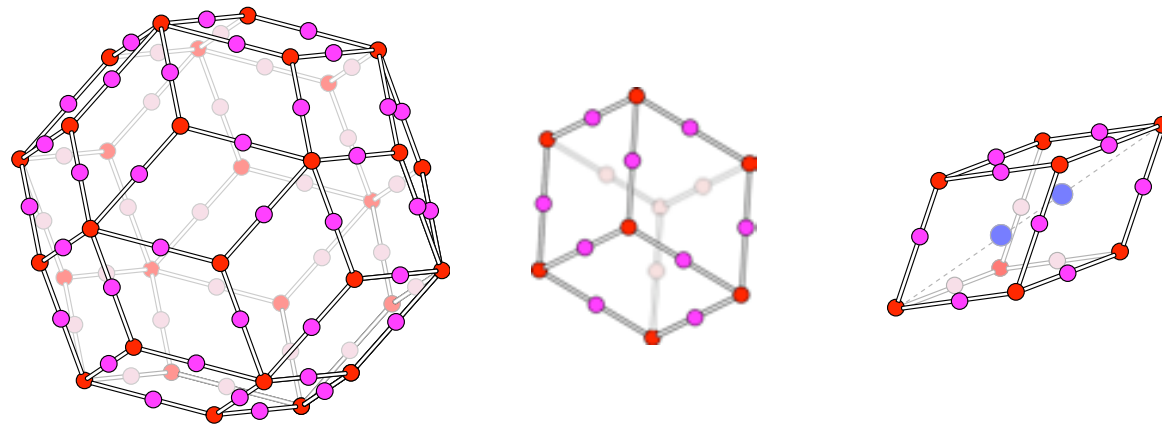
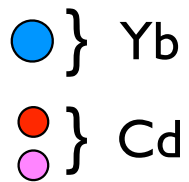
**OR**



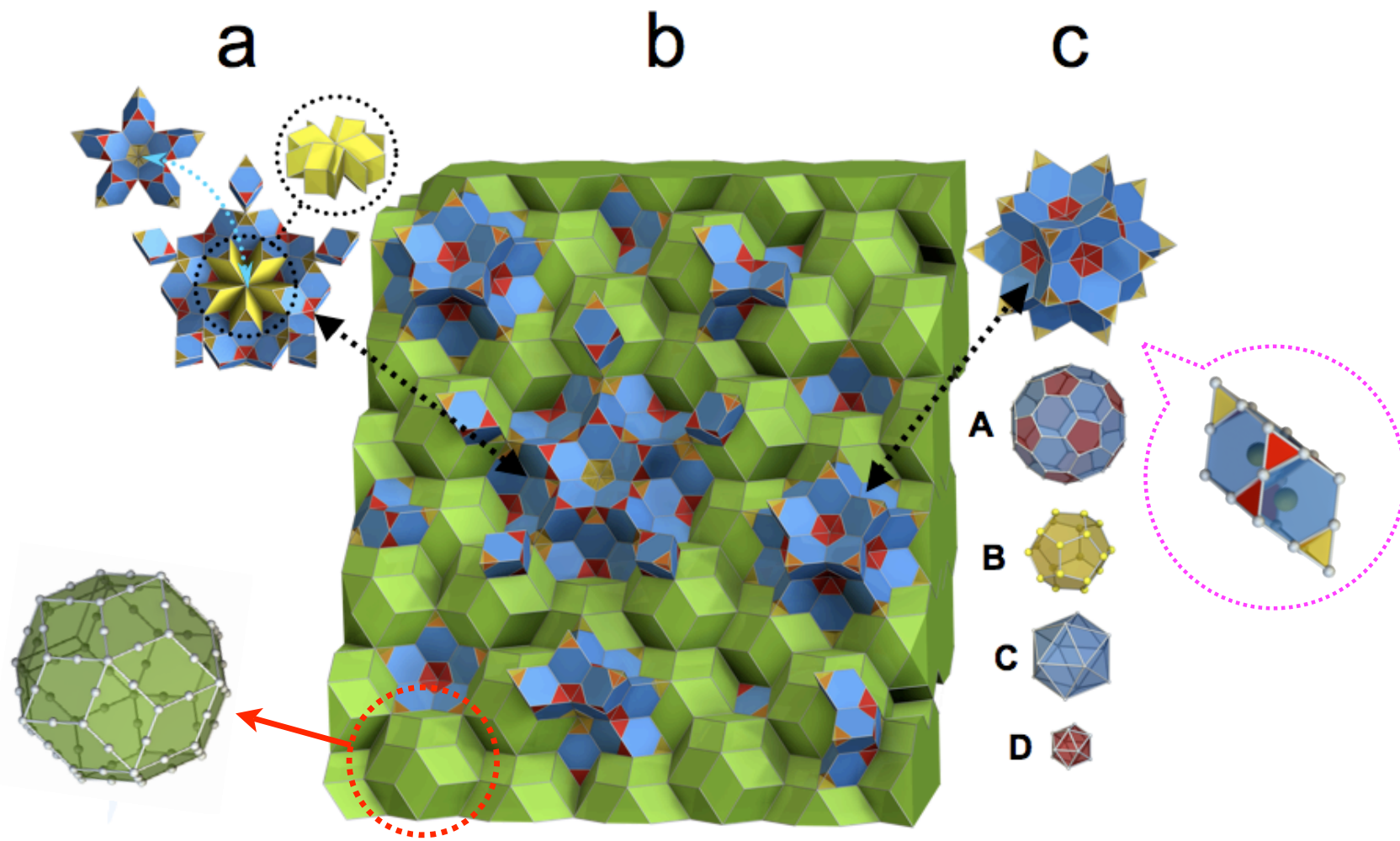
**AR**

# Atomic decorations of the building units

i-Yb-Cd



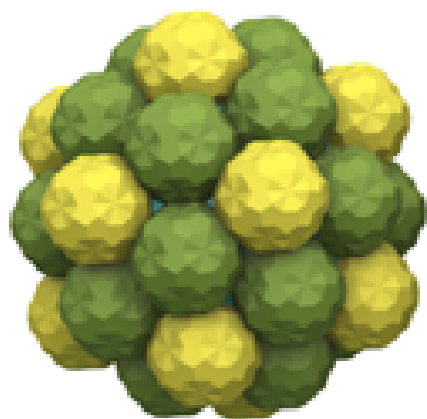
# Space filling i-Yb-Cd QC structure represented by using the building units



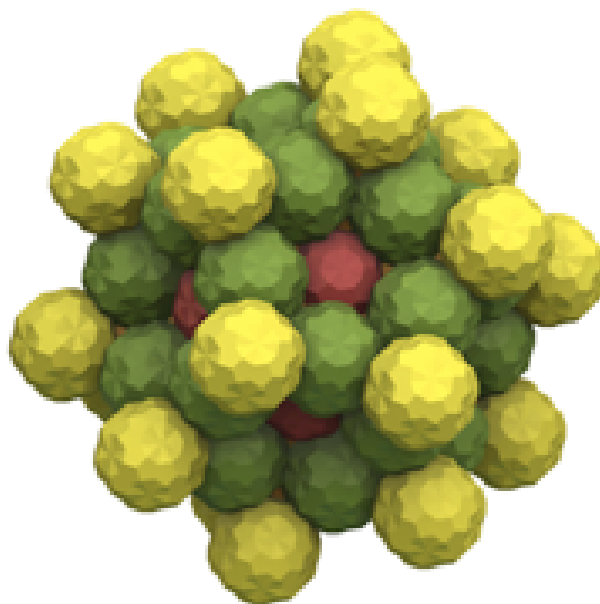


# 6D structure and 3D structure

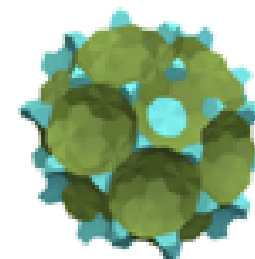
# 6D structure model of i-YbCd



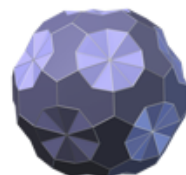
V:(000000)









B:(111111)/2



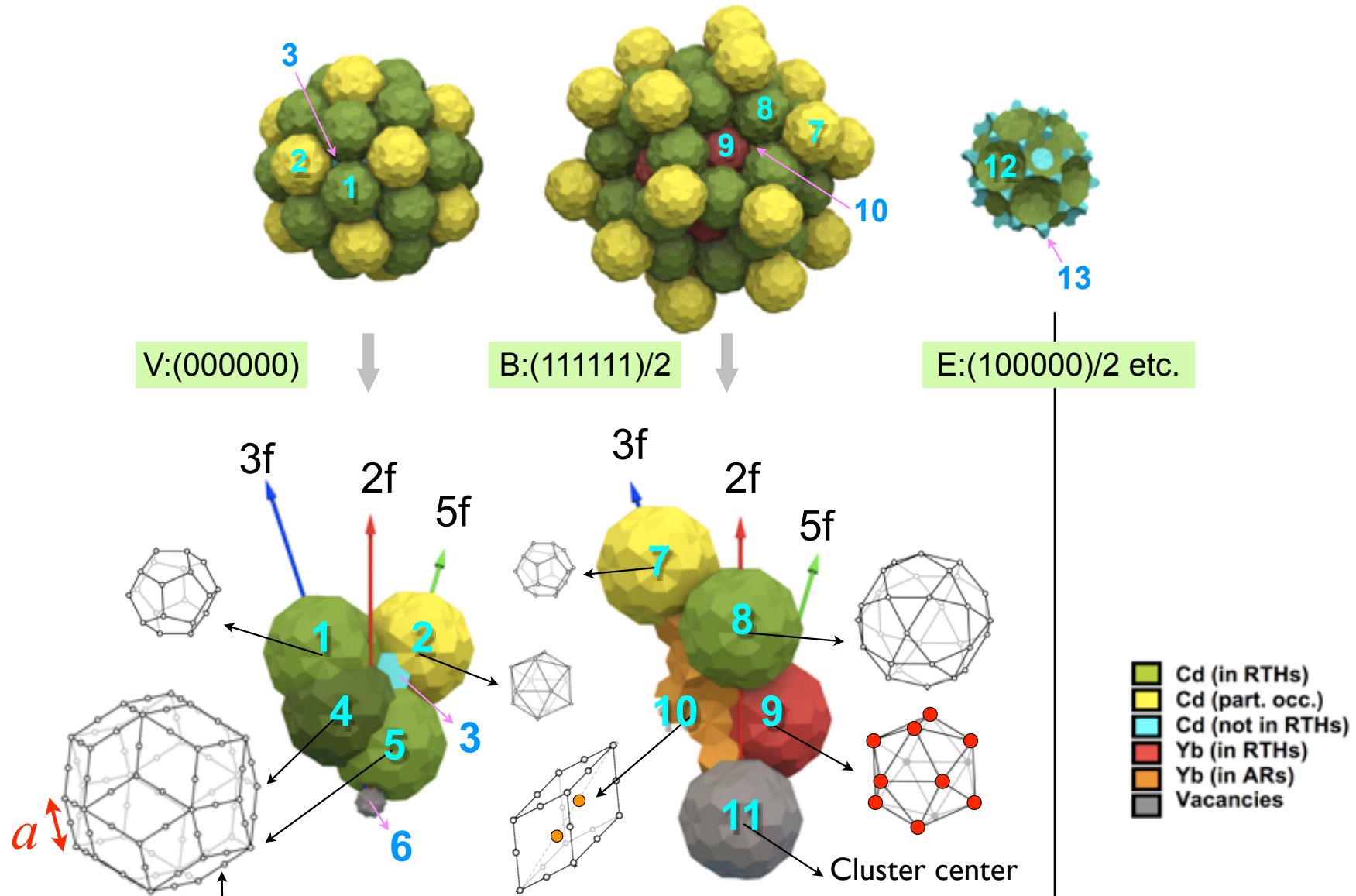
E:(100000)/2



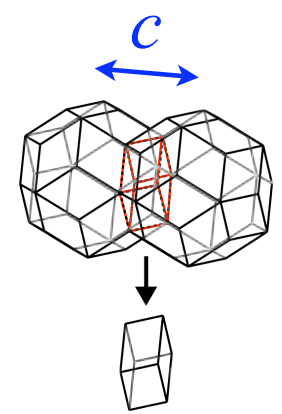
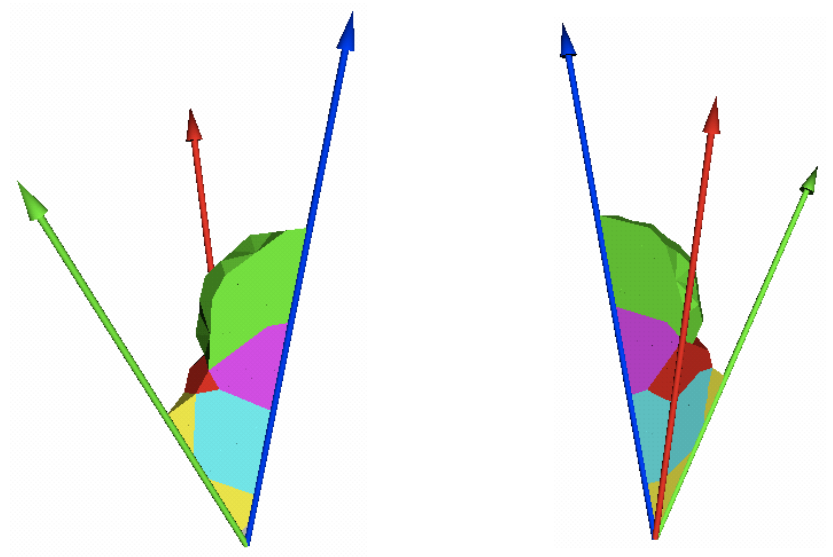
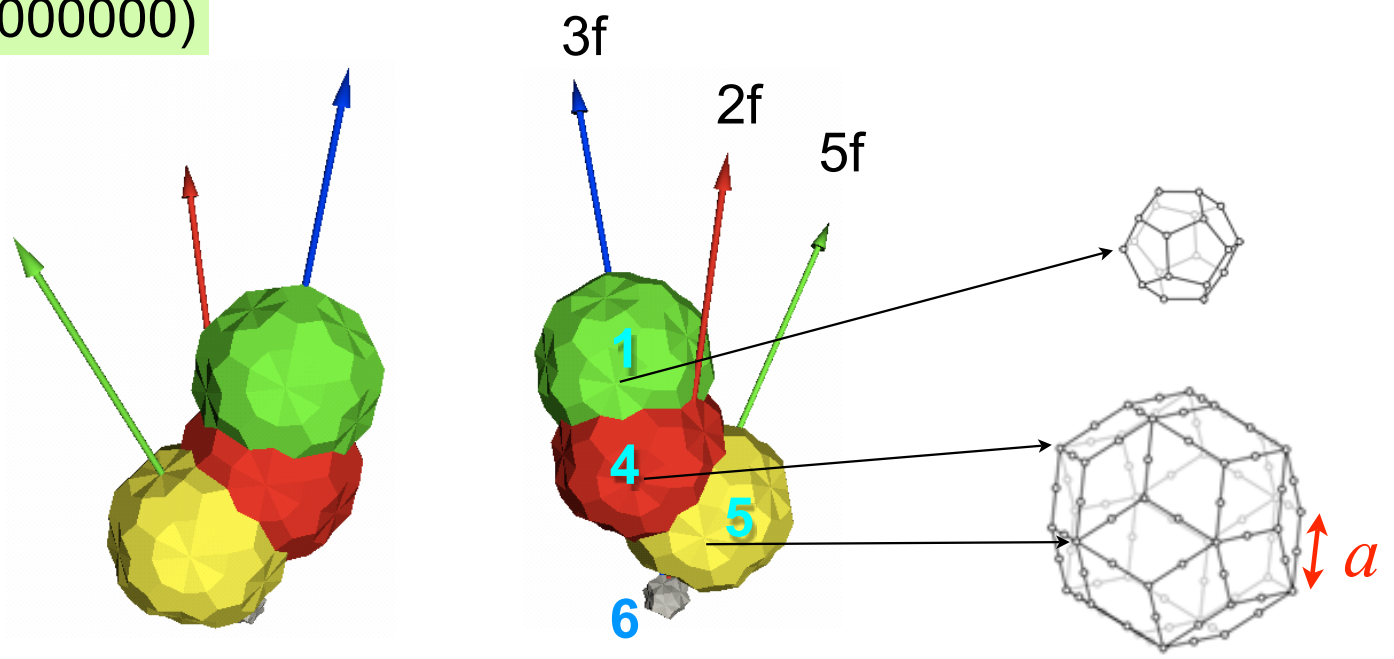
:OD for the 12-fold vertices of 3DPT

-  Cd (in RTHs)
-  Cd (part. occ.)
-  Cd (not in RTHs)
-  Yb (in RTHs)
-  Yb (in ARs)
-  Vacancies

# 6D structure model of i-YbCd (cont.)

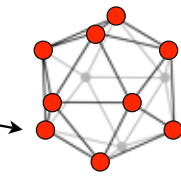
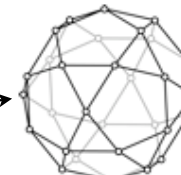
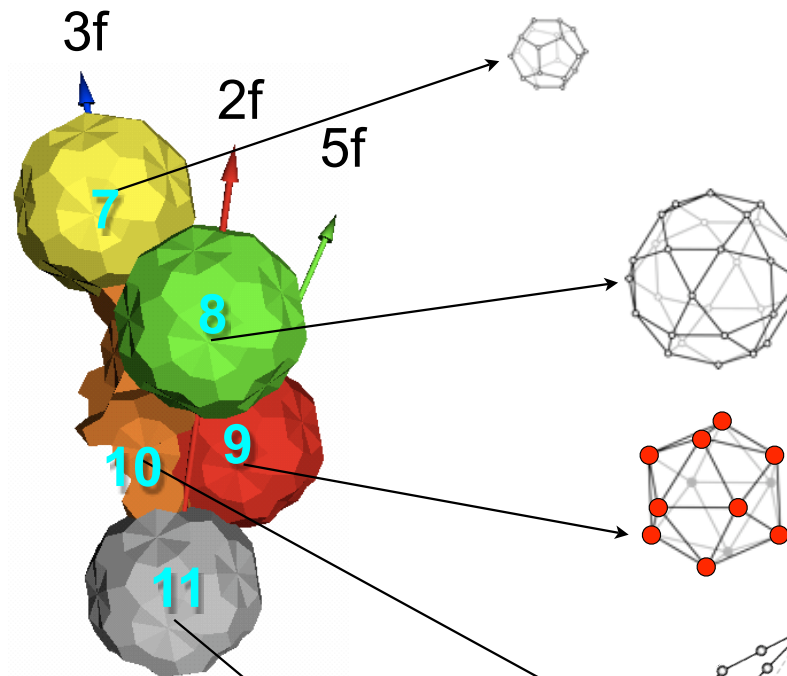
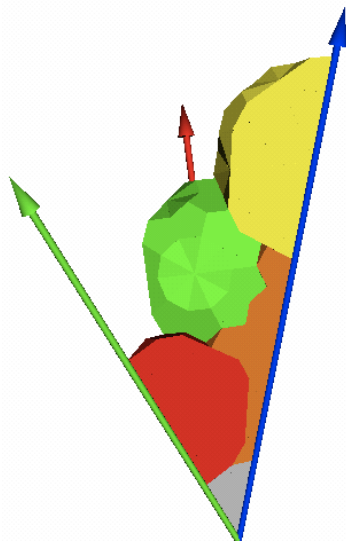
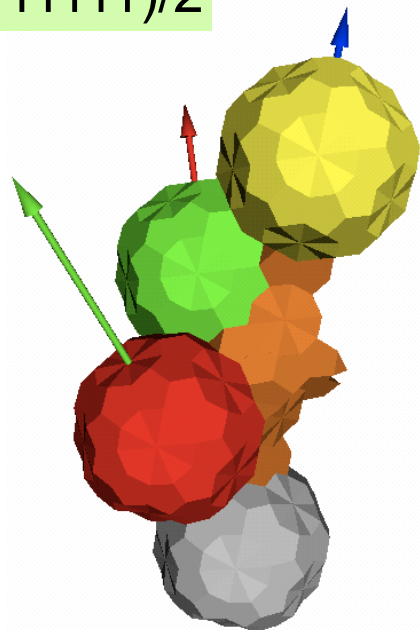


V:(000000)

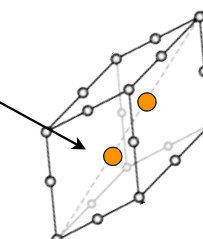


The c-link imposes a geometric constraint for shell structures.

B:(111111)/2



**Yb** 68.6%  
5.80Å

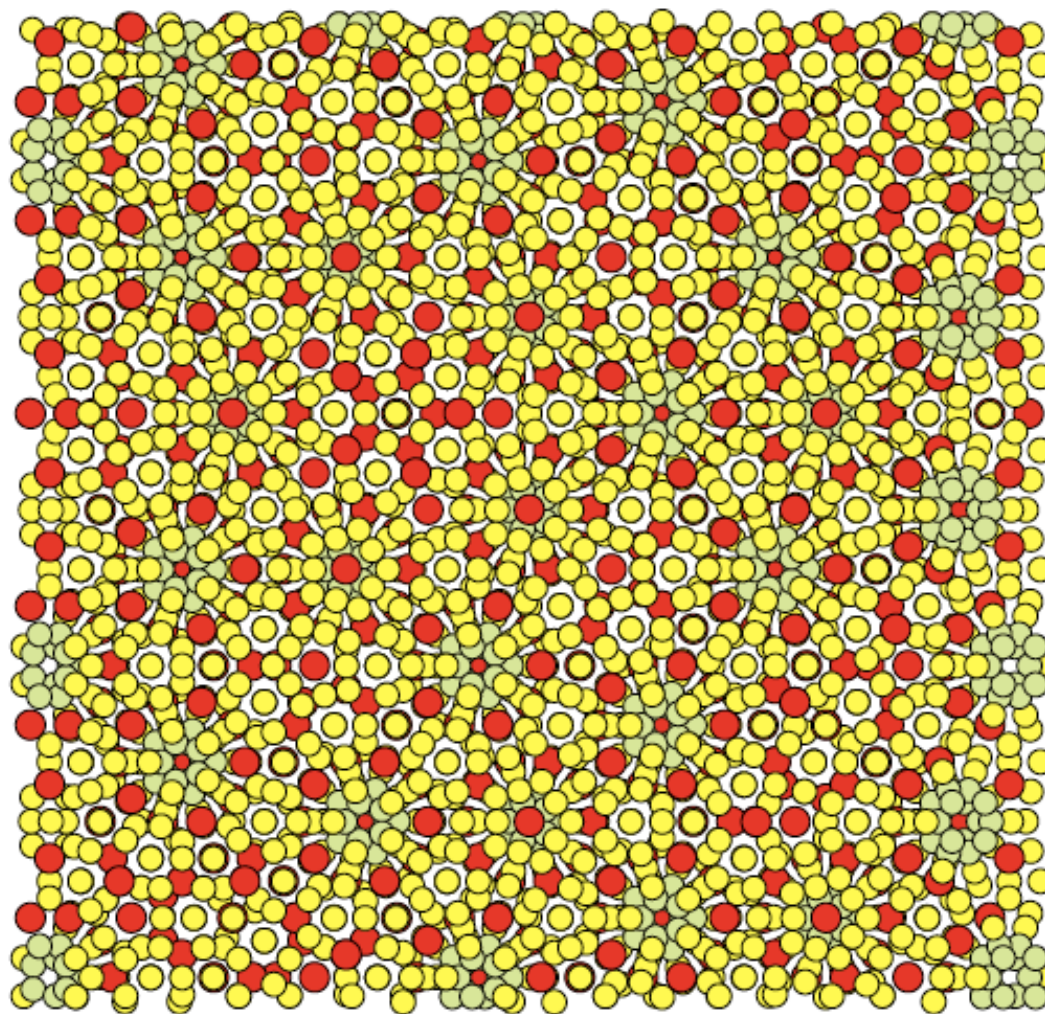


**Yb** 31.4%  
3.52Å

RT cluster center

(Twelve-fold vertices of 3DPT)

# Cross section structure of Yb-Cd i-QC normal to a five-fold axis

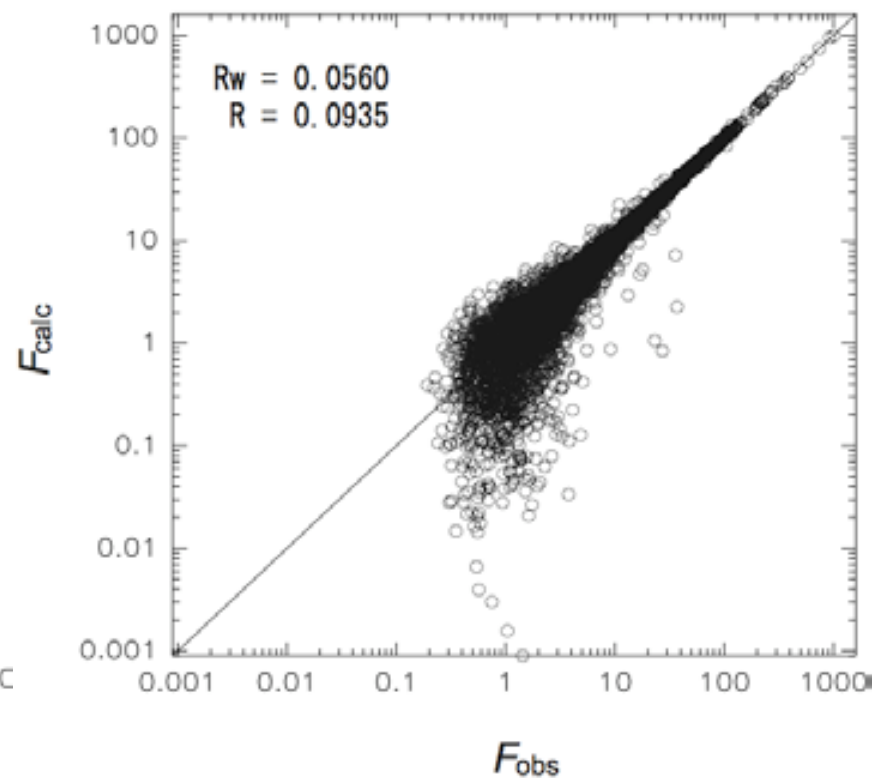
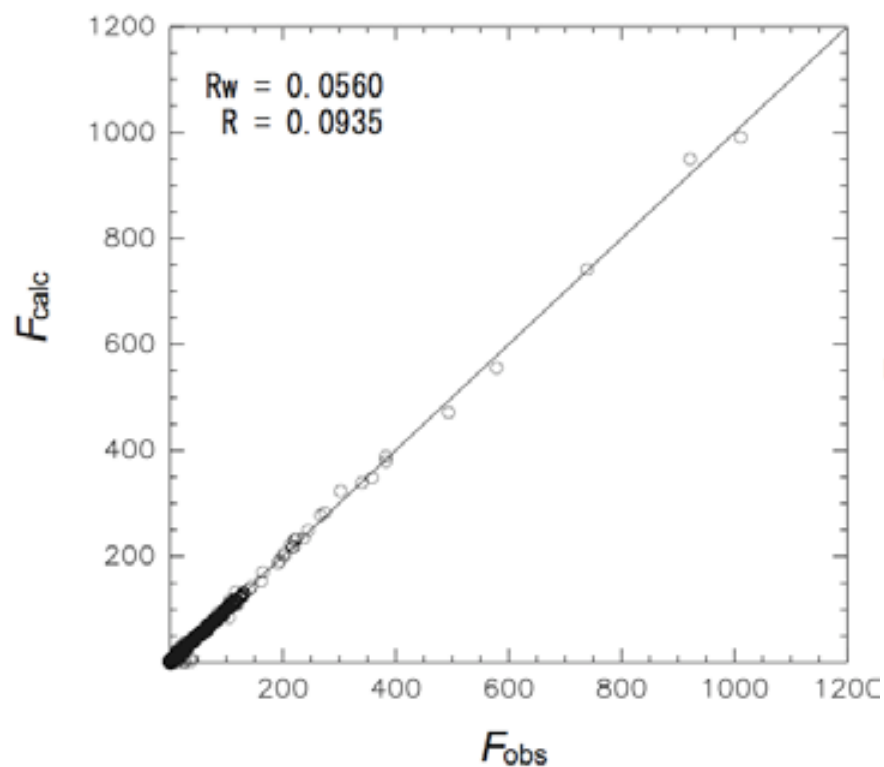


# Refined structure model of YbCd i-QC

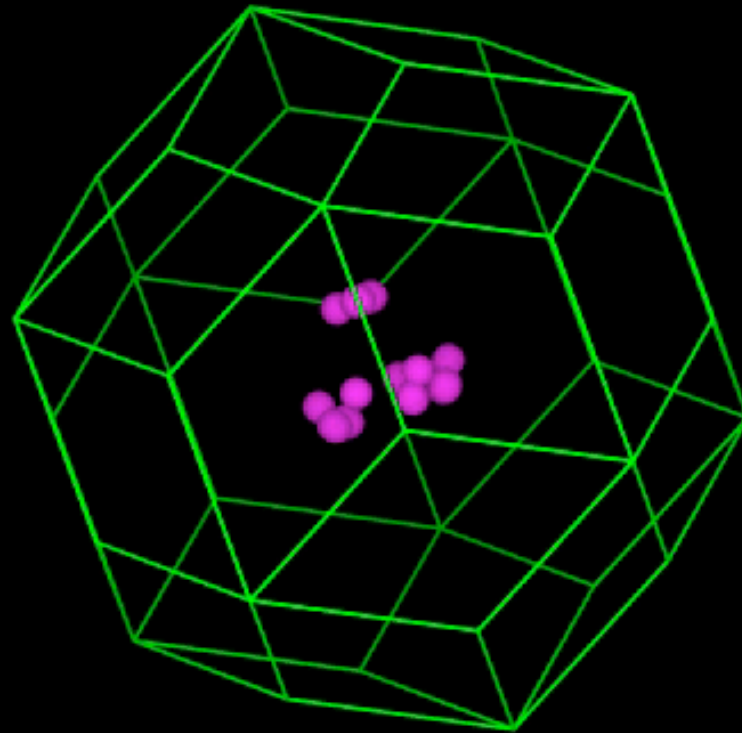
# Refinement of the i-Yb-Cd model

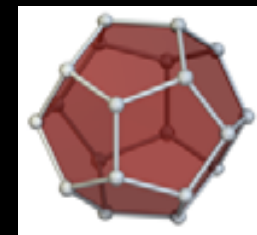
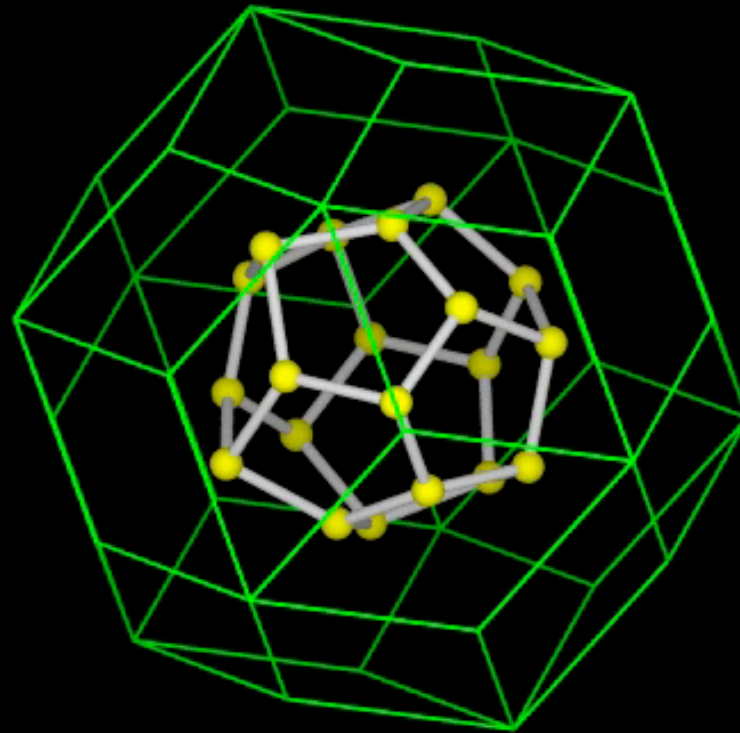
5024 reflections

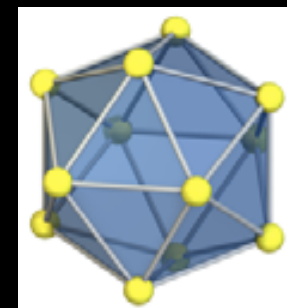
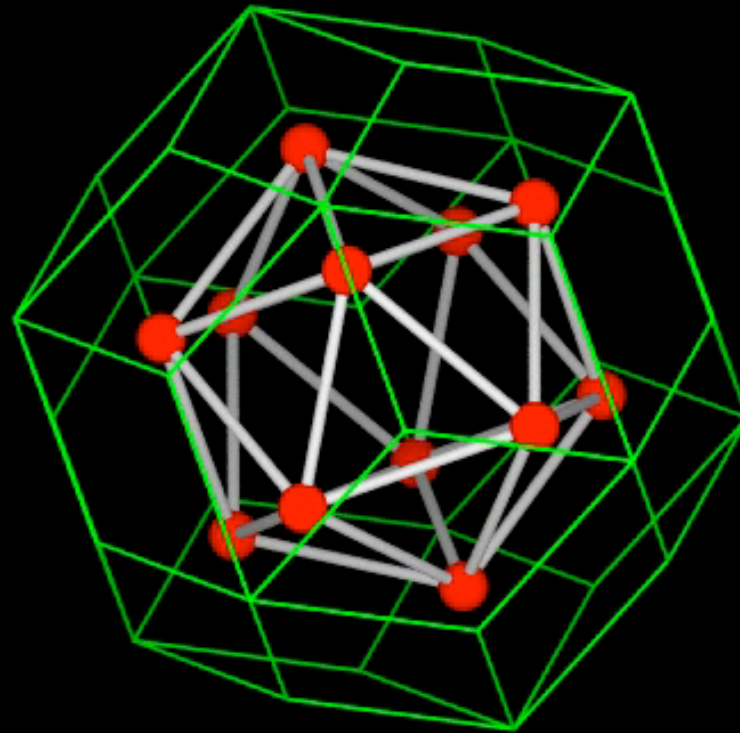
251 refined parameters

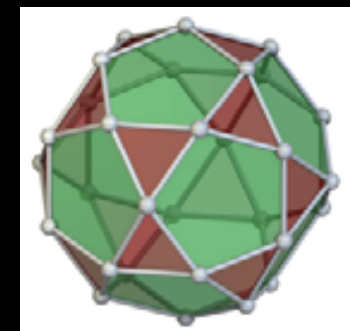
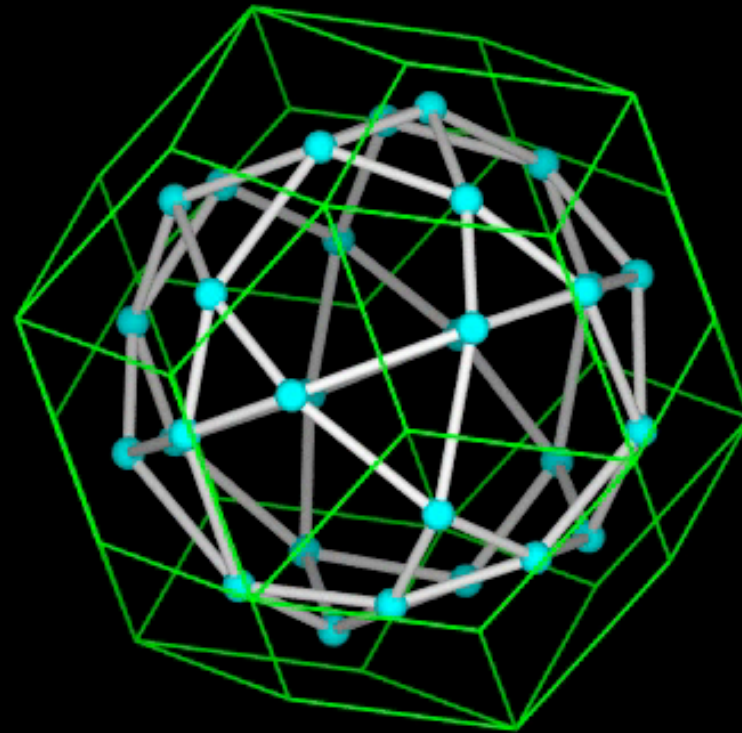


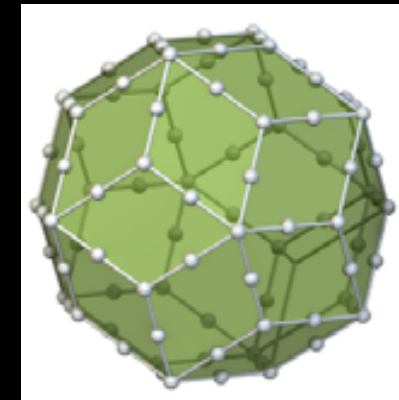
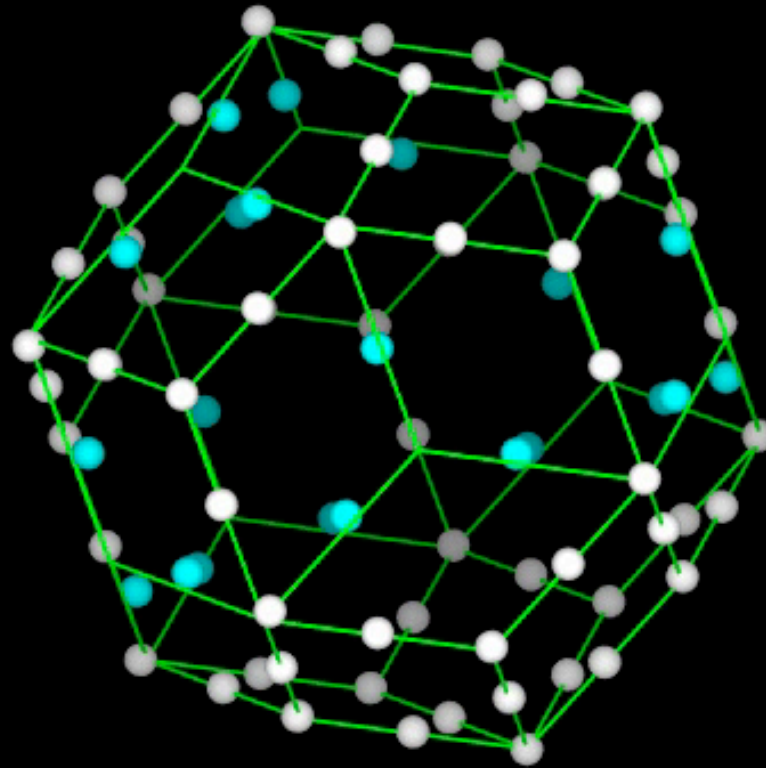


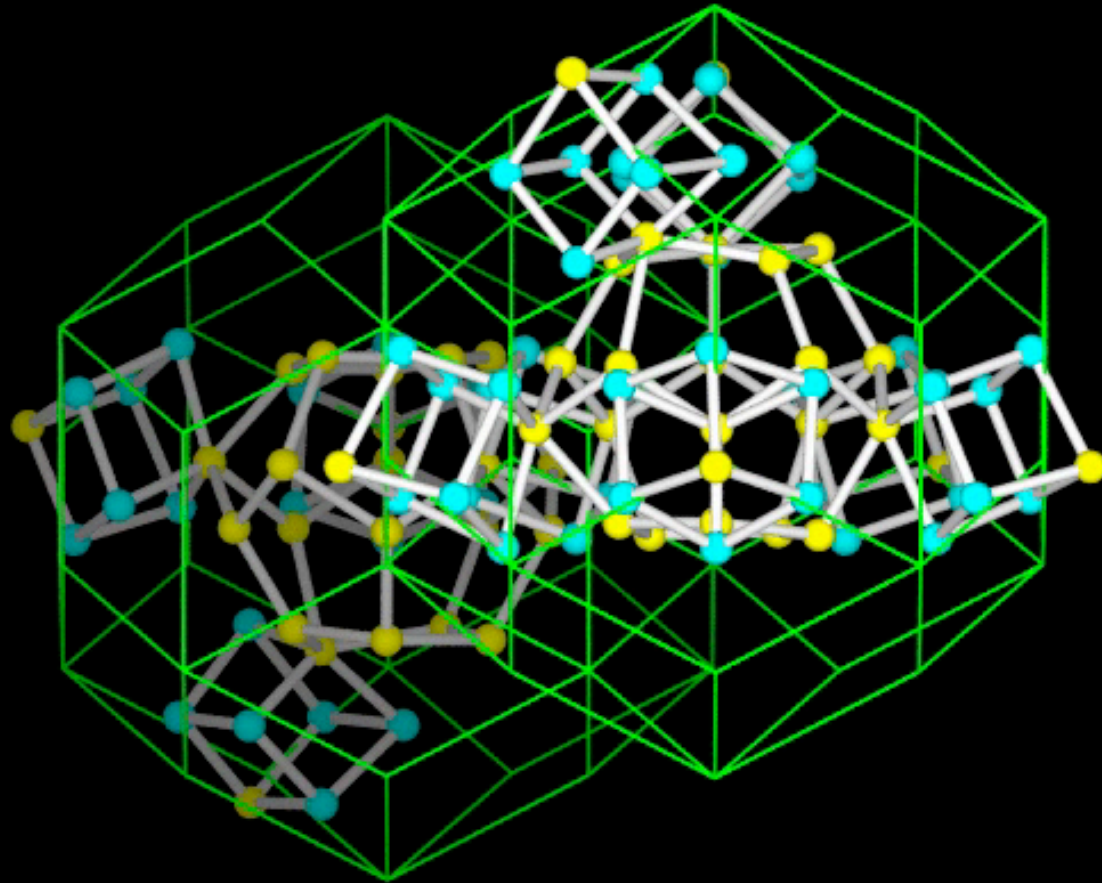


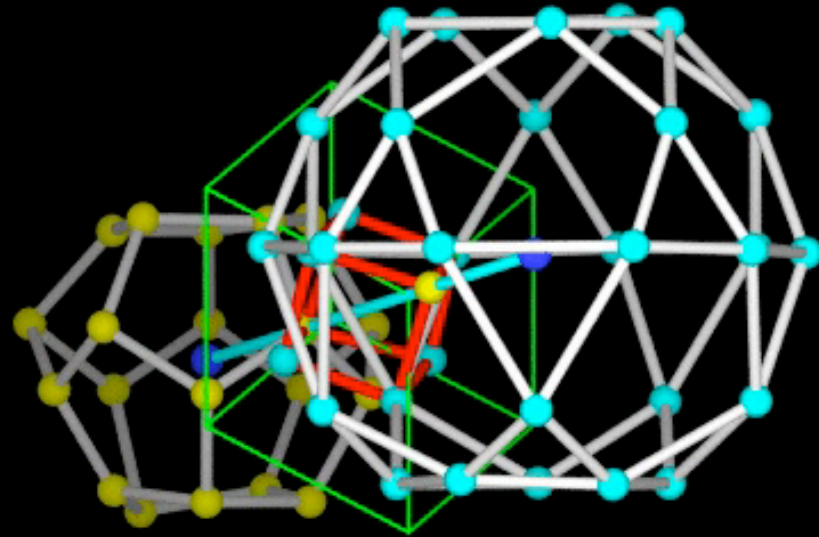




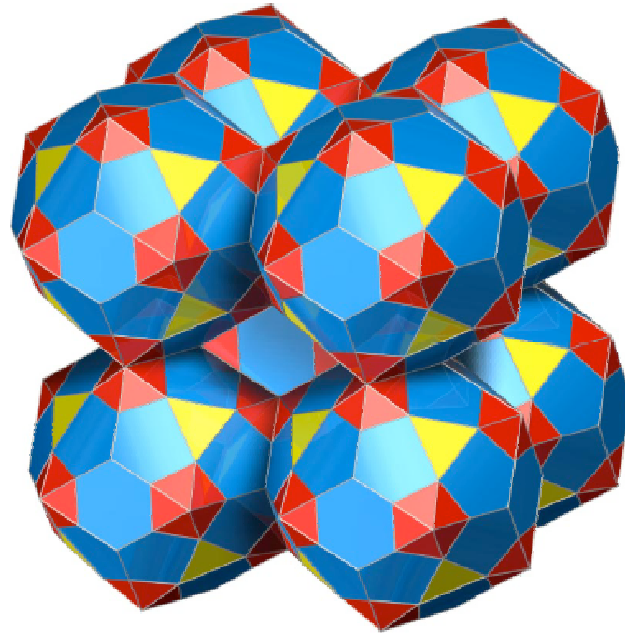








## RT cluster description of 1/1 approximant crystal





# Summary

- RT cluster is the common largest building unit in approximant crystals and quasicrystal of i-YbCd.
- *b*- and *c*- links connect RT clusters.
- RT, AR and OR units are the necessary building units for the space filling structure model of i-Yb-Cd.
- The *c*- link is a possible source of chemical order in a ternary Yb-Cd type QC's.
- Refined structure model of i-Yb-Cd QC reproduces the characteristic feature of RT cluster that is found in approximant crystals.