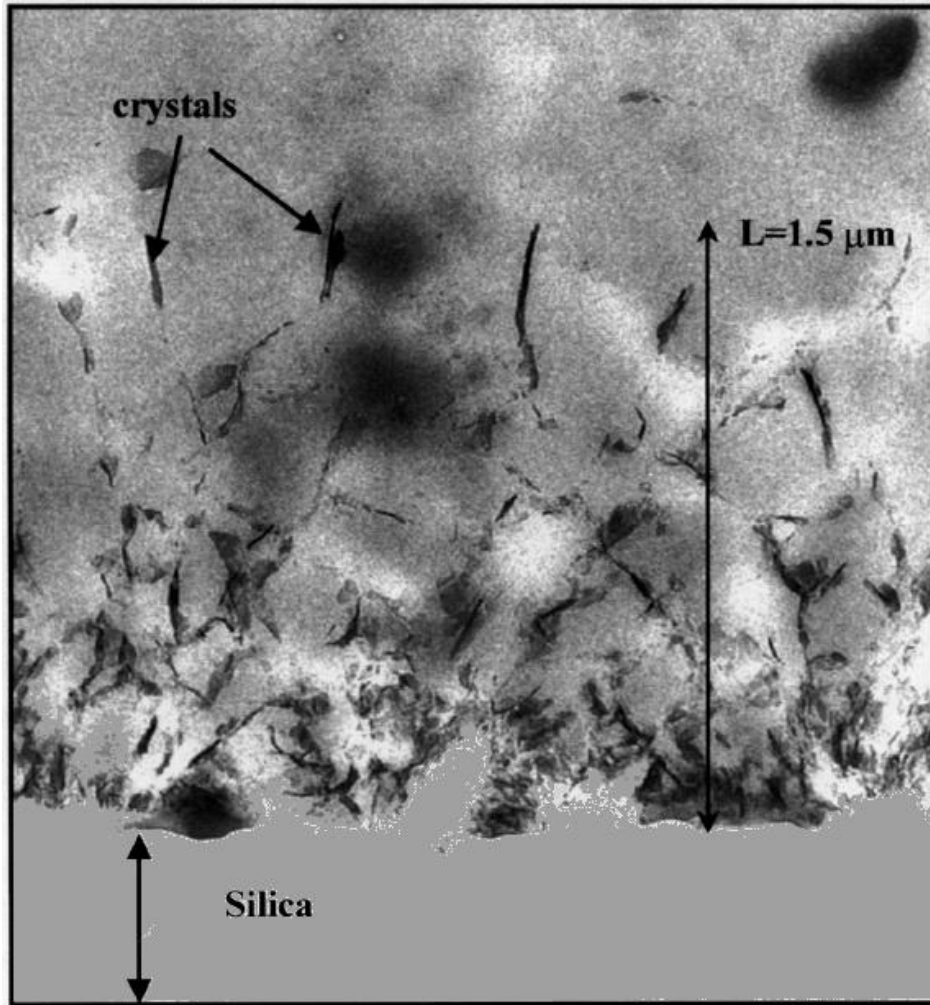


Density functional molecular dynamics simulations of hydroxy apatite nucleation on silica based glass surfaces

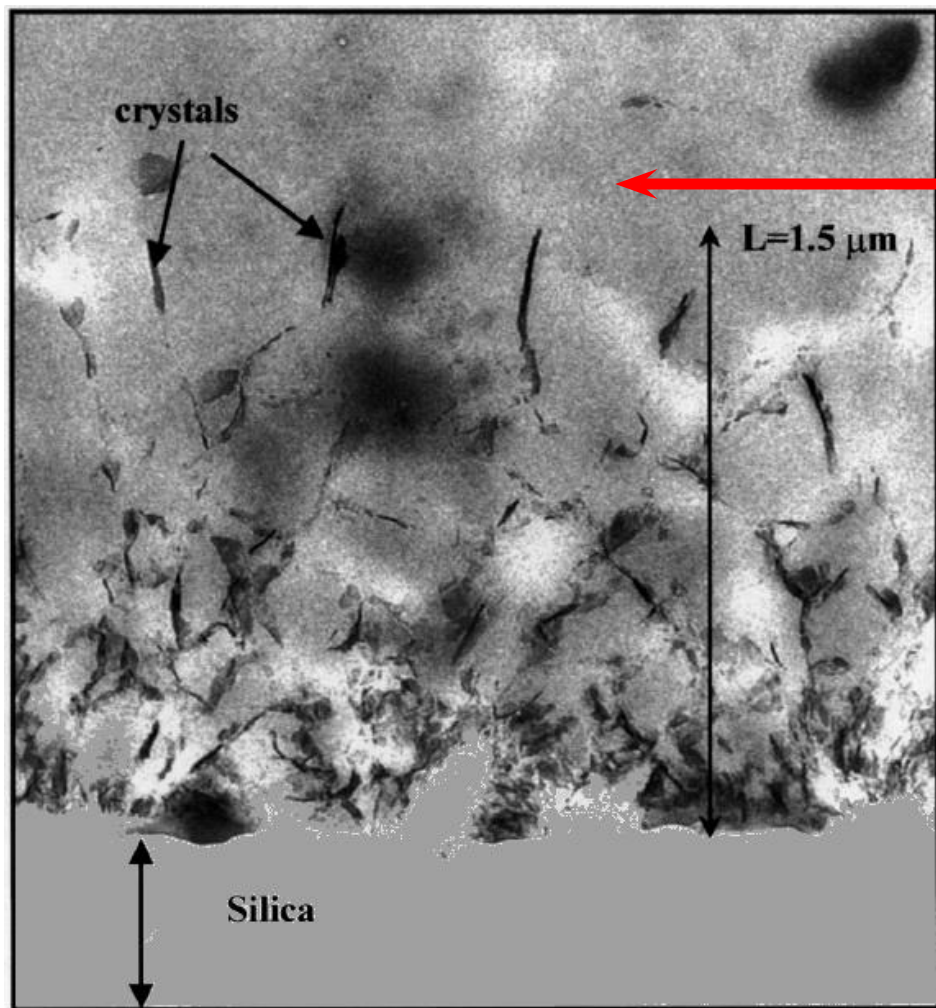
SNF project 21-63795.00

René Windiks

Paul Scherrer Institute, Villigen PSI, Switzerland



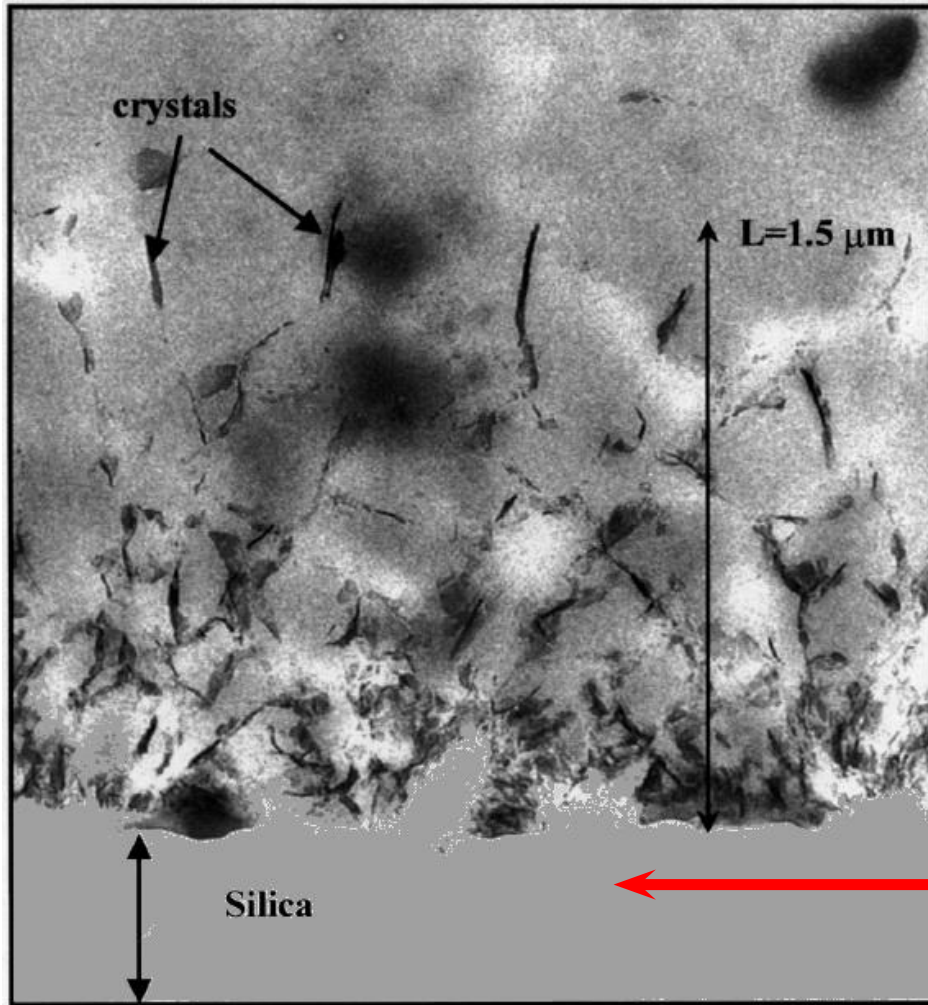
transversal TEM image of HAC on SiO_2 glass
Ngankam *et al.* *J. Cryst. Growth* (1999)



hydroxy apatite (HAC), amorphous,
 $\text{Ca}_5(\text{PO}_4)_3\text{OH}$

- one of the major compounds of mammalian bone
- model compound for calcified tissues
- phosphate species at pH 7.4:
 HPO_4^{2-}

transversal TEM image of HAC on SiO_2 glass
Ngankam *et al.* *J. Cryst. Growth* (1999)

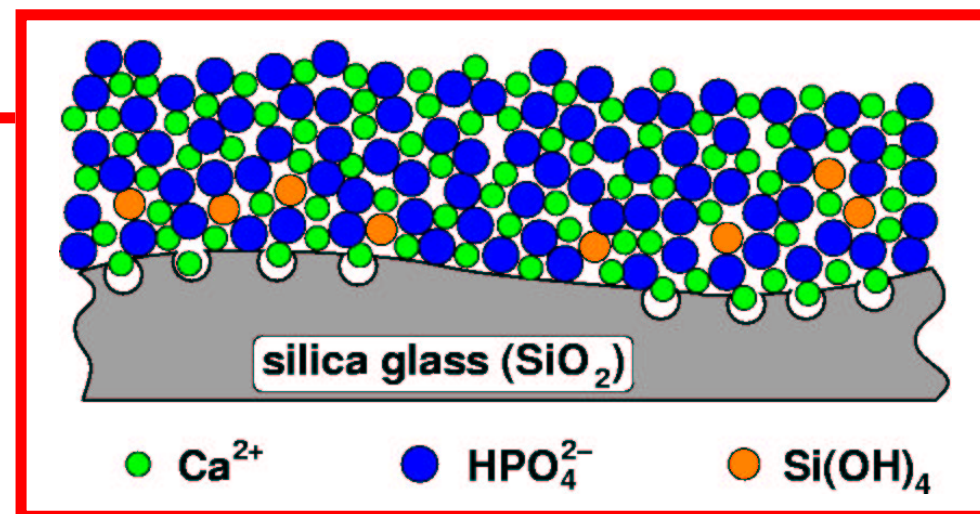
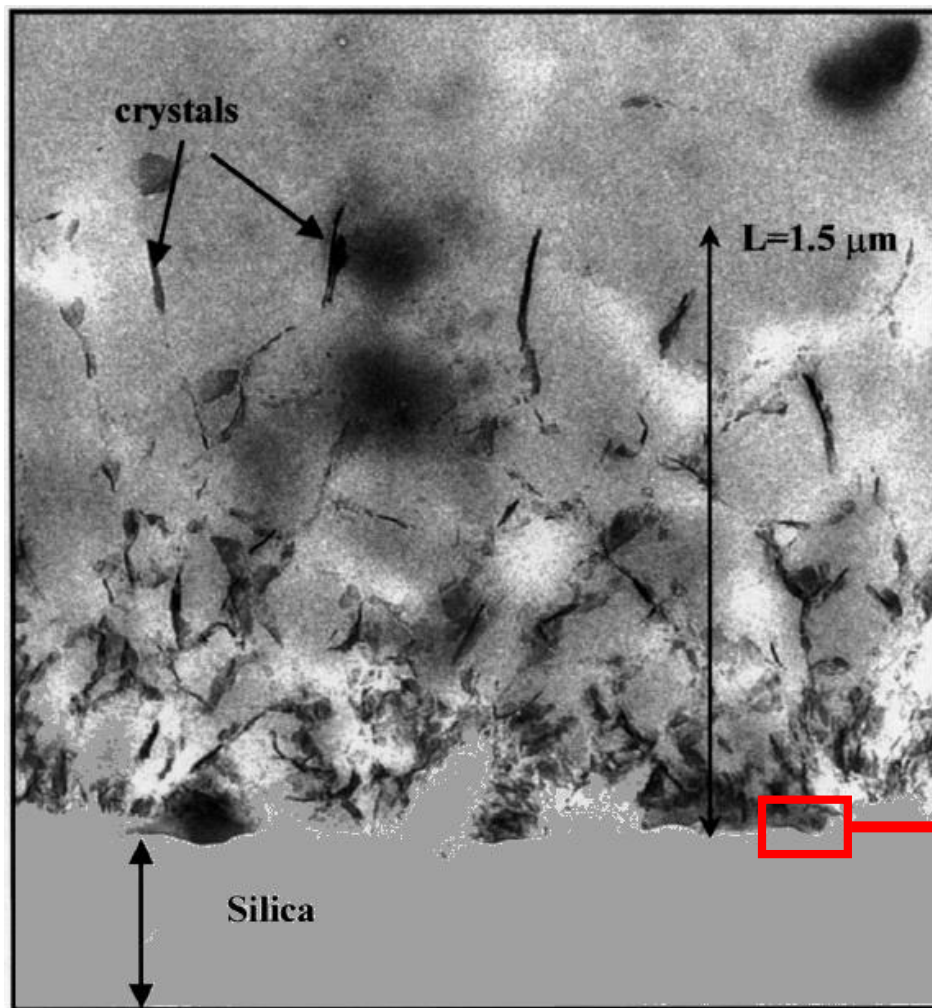


transversal TEM image of HAC on SiO_2 glass
Ngankam *et al.* *J. Cryst. Growth* (1999)

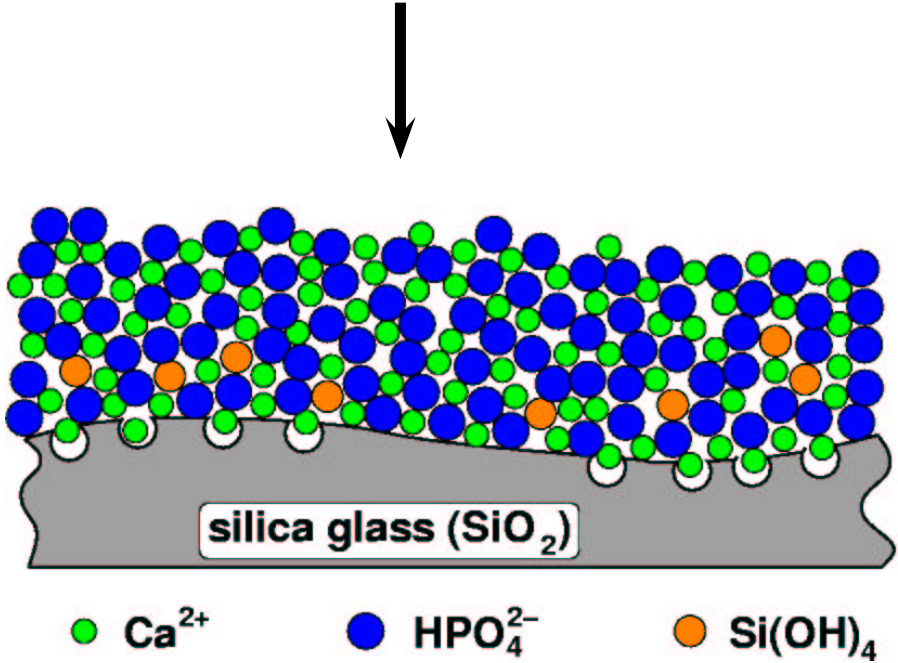
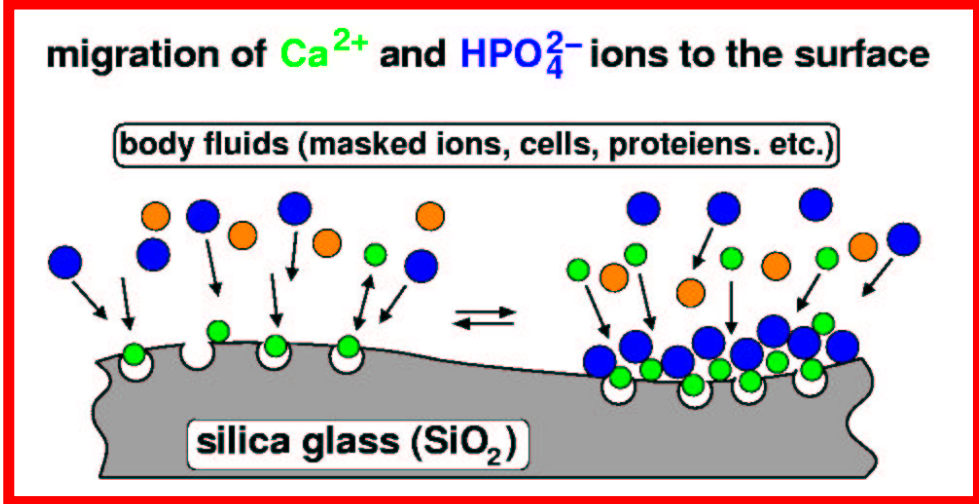
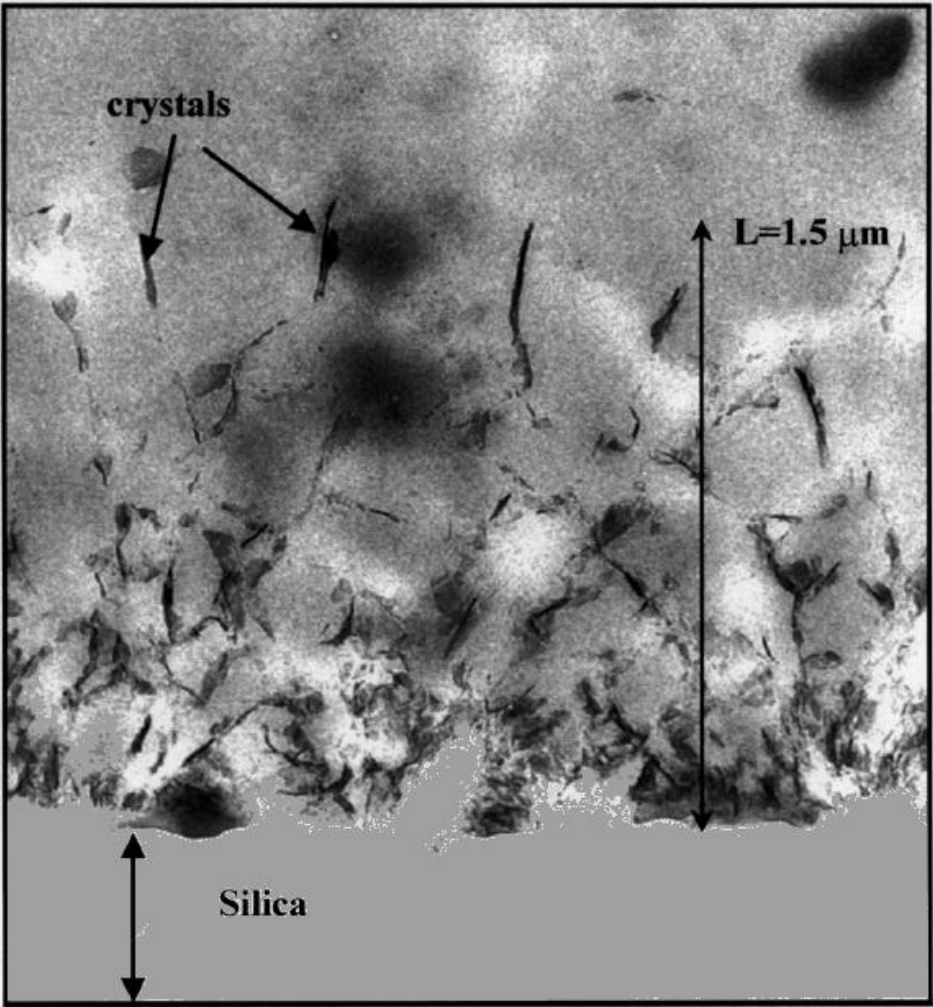
silica glass, SiO_2

- 3D network of corner- and edge-sharing $\text{SiO}_{4/2}$ tetrahedra
- disordered system, contains defects
- initiate the formation of HAC on its surface → bioactive material
- forms strong connection to natural bone
- used for prosthetic bones, dental implants

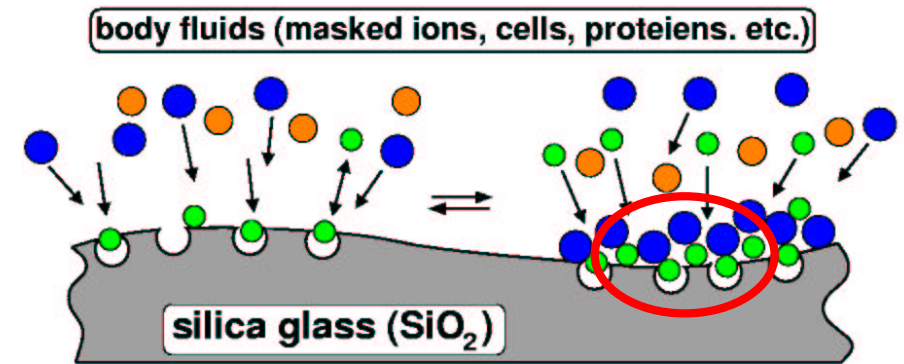
Hydroxy apatite coated silica surface



Hydroxy apatite nucleation



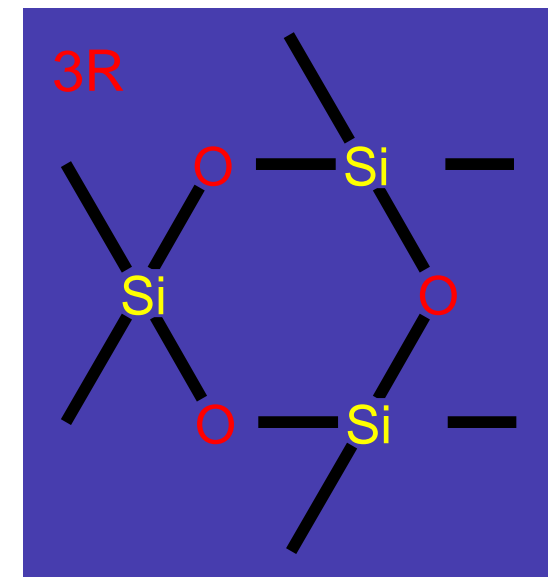
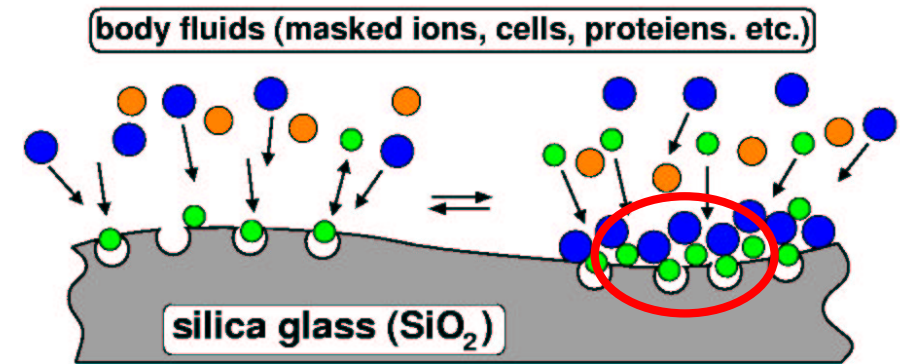
migration of Ca^{2+} and HPO_4^{2-} ions to the surface



■ facts

- ◆ surface $\equiv\text{SiOH}$ and $=\text{Si}(\text{OH})_2$ are important
- ◆ Ca and phosphate ion complexation onto **3R** silica rings (defect site)

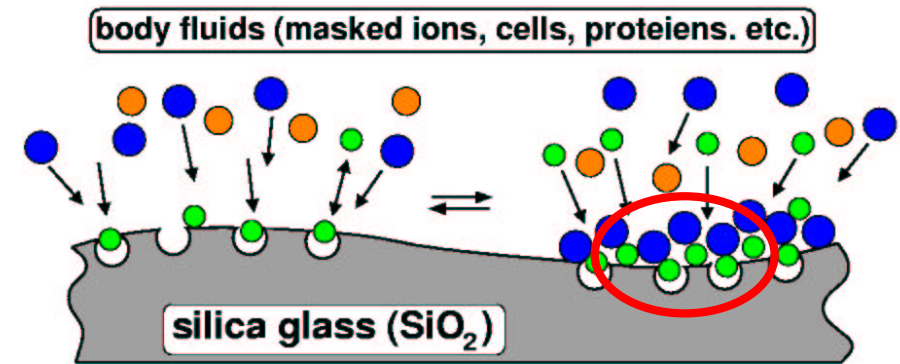
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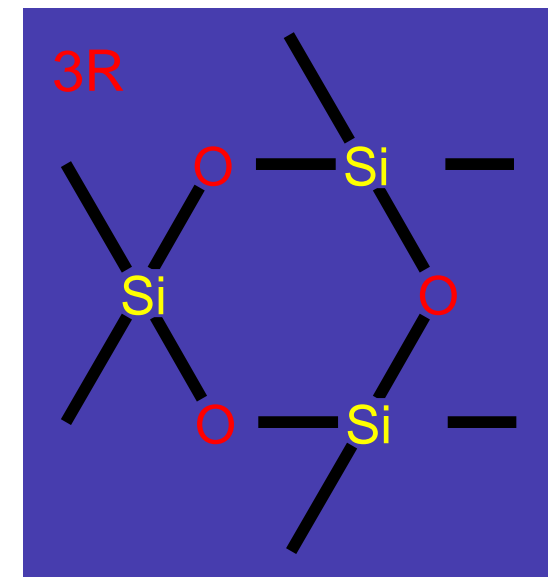
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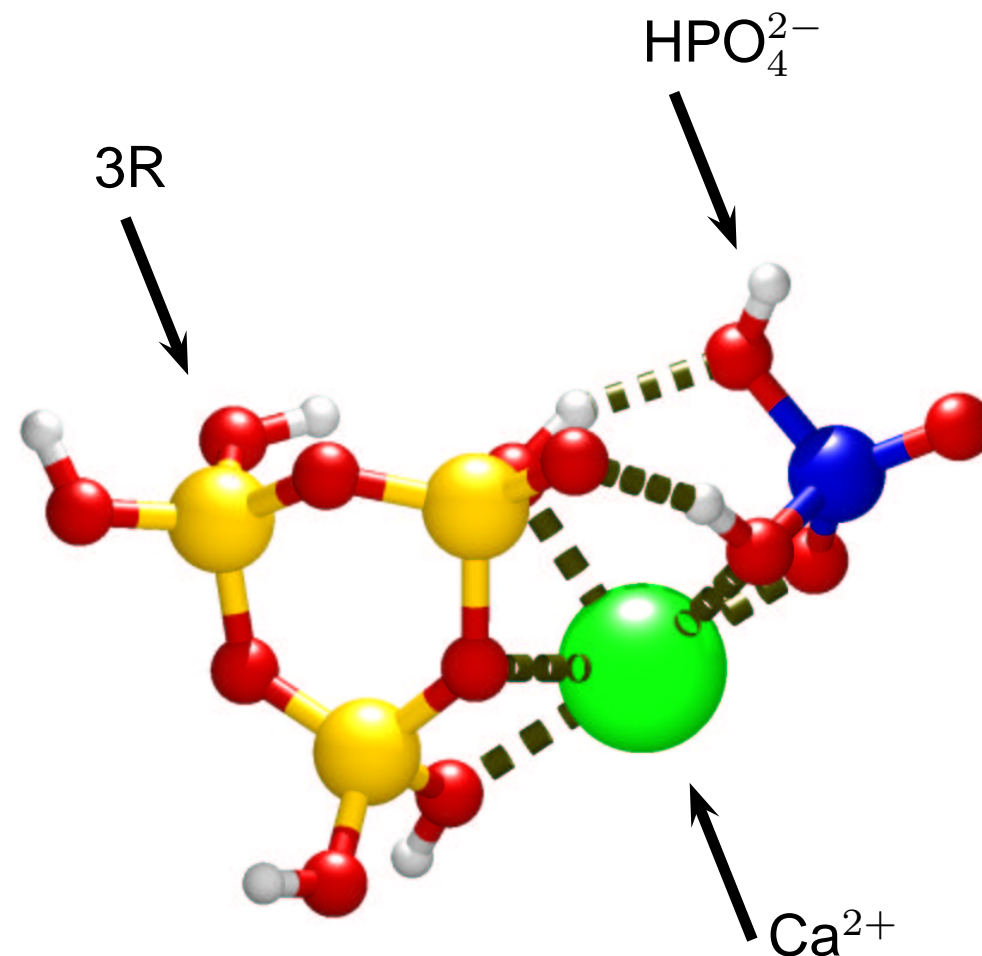


■ open questions:

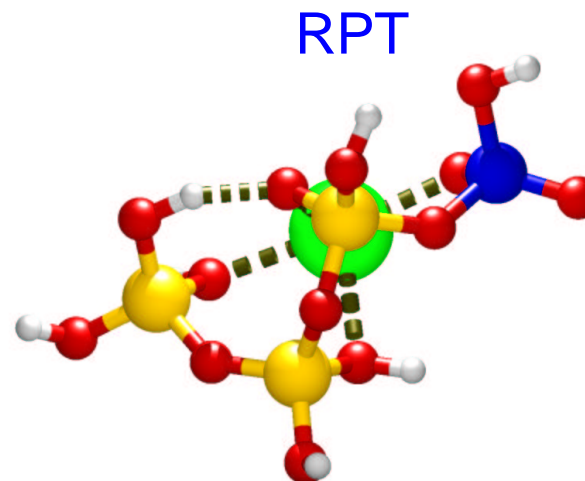
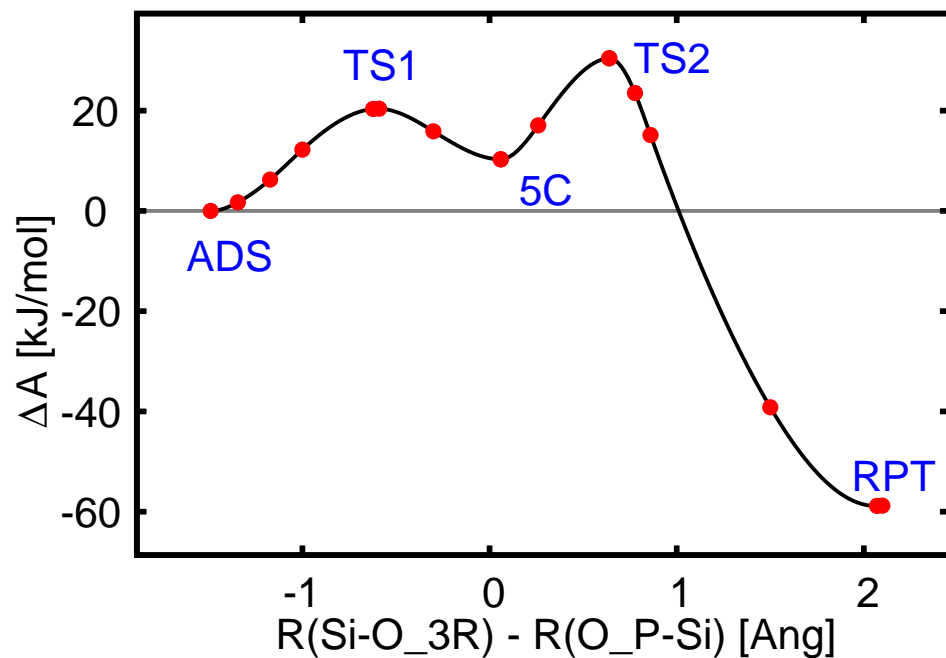
- ◆ types of Ca and phosphate surface complexes ?
- ◆ stabilization by hydrogen bonds only or also formation of Si-O-P linkages ?
- ◆ rupture of **3R** ?



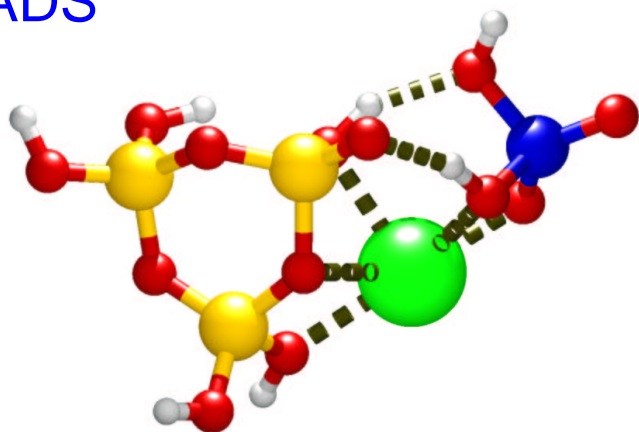
- knowledge of simple model systems provides important conceptual information
- computational tools:
 - ◆ density functional methods (DMol³, B. Delley)
 - ◆ static structure optimizations
 - ◆ molecular dynamics simulations (simulated annealing, constrained MD)



Free energy profile



ADS



5C

