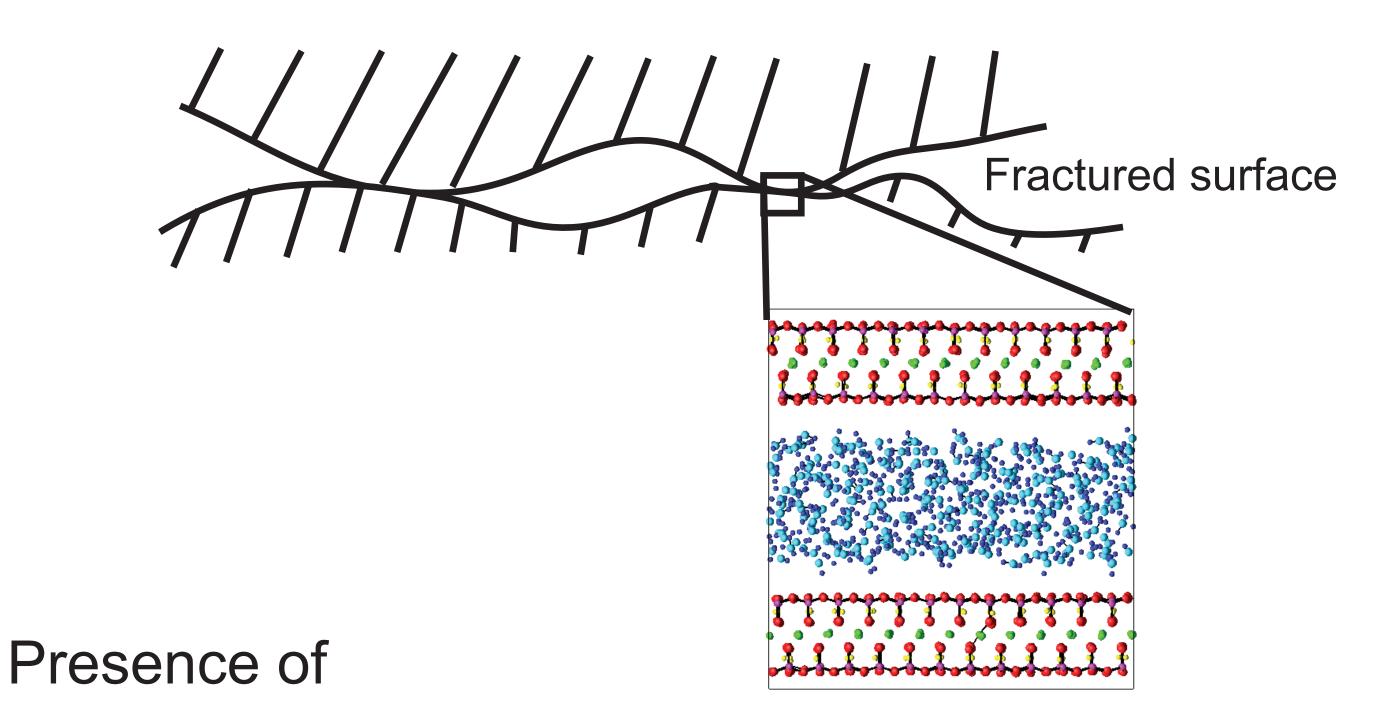
Structure of mineral/water interfaces in geoscience

Hiroshi SAKUMA

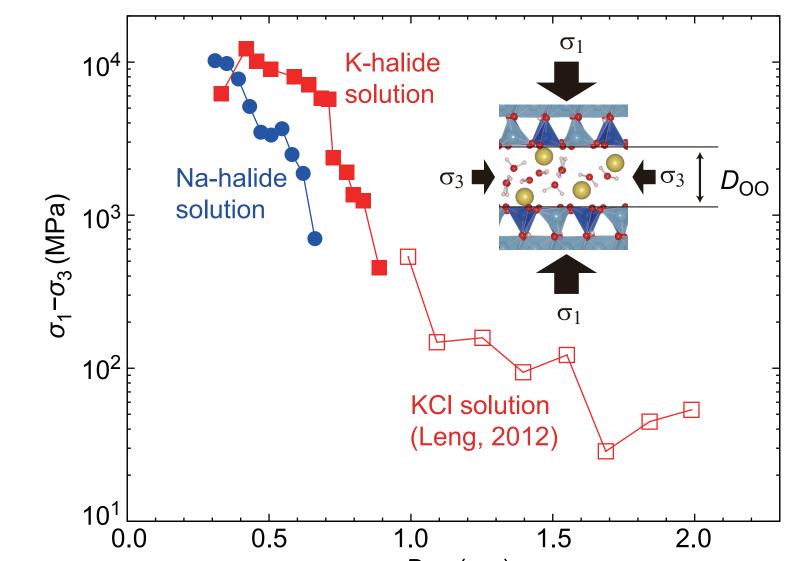
National Institute for Materials Science (SAKUMA.Hiroshi@nims.go.jp)

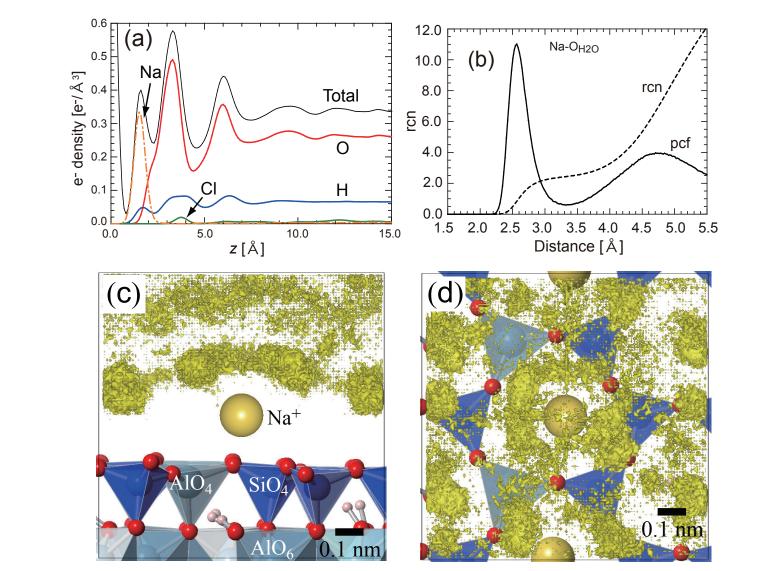
Effect of water on rock friction



1. Inhibition of direct contact of mineral surfaces Repulsive hydration force

Strong interaction between adsorbed water and ions on a charged mineral surface





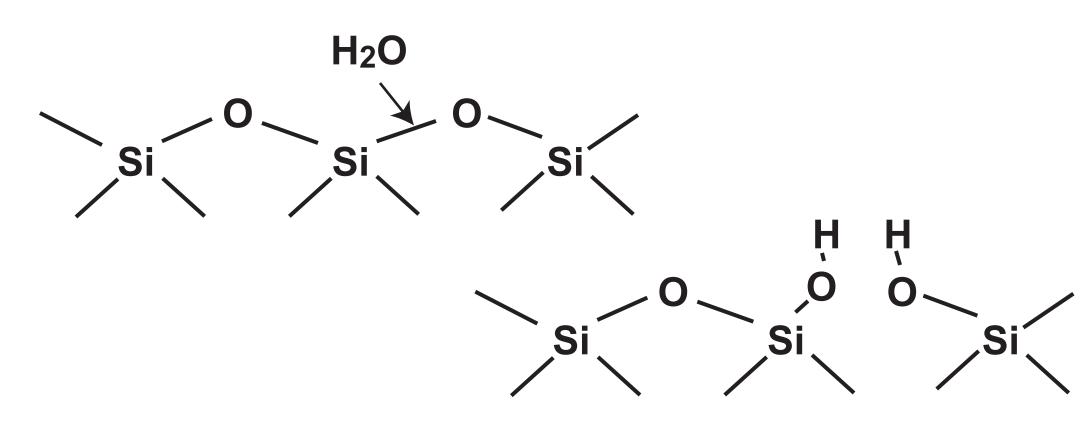
adsorbed water molecules

makes frictional strength weak due to

- 1. Inhibition of direct contact of mineral surfaces
- 2. Lubrication
- 3. Chemical weakening

3. Chemical weakening

Adsorbed water may assist chemical reaction at real contact area under applied normal load.



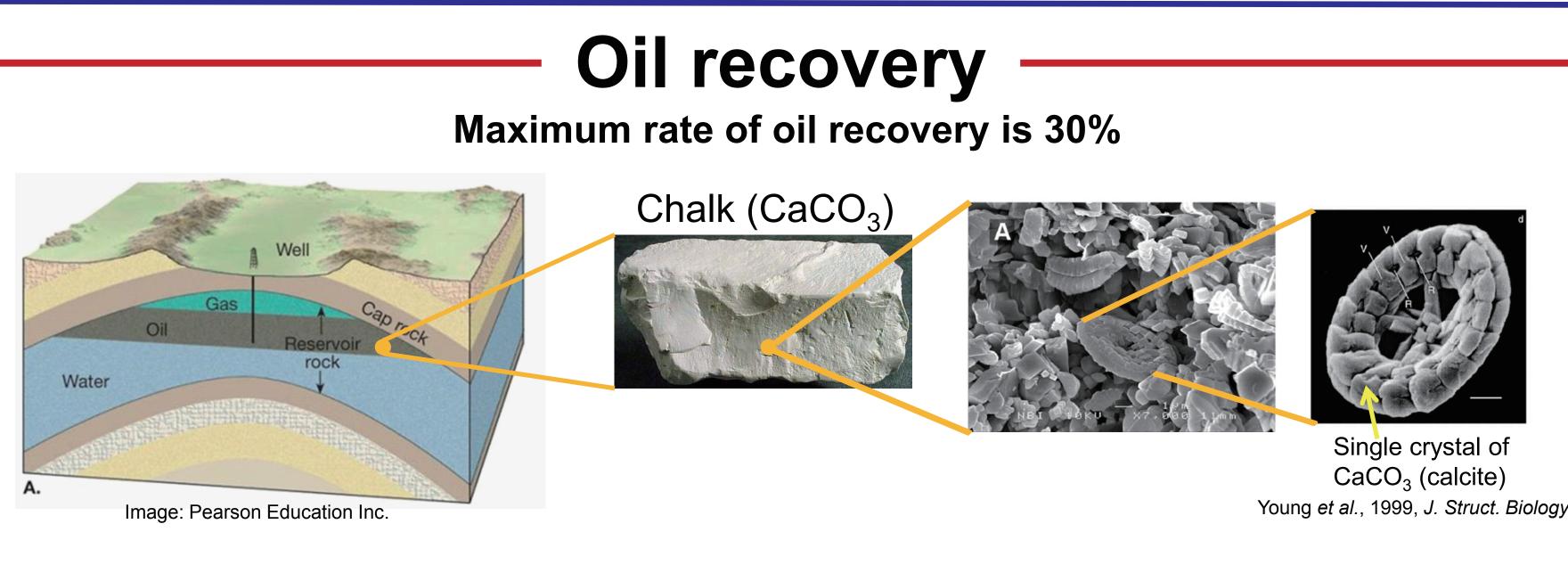
Can we observe the equilibrium structure at real contact area under applied normal load?

 $D_{OO}(nm)$

Differential compressive stress to remove adsorbed water between mica surfaces (Sakuma, 2013)

Isodensity profiles of water on a muscovite mica surface (Sakuma et al., 2011)

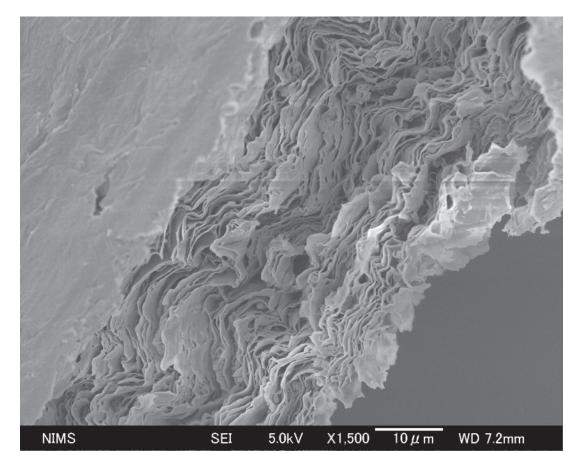
Interfacial structure is important for estimating the hydration force.



Wettability alteration of mineral surfaces

Structure of mienral surface is important !

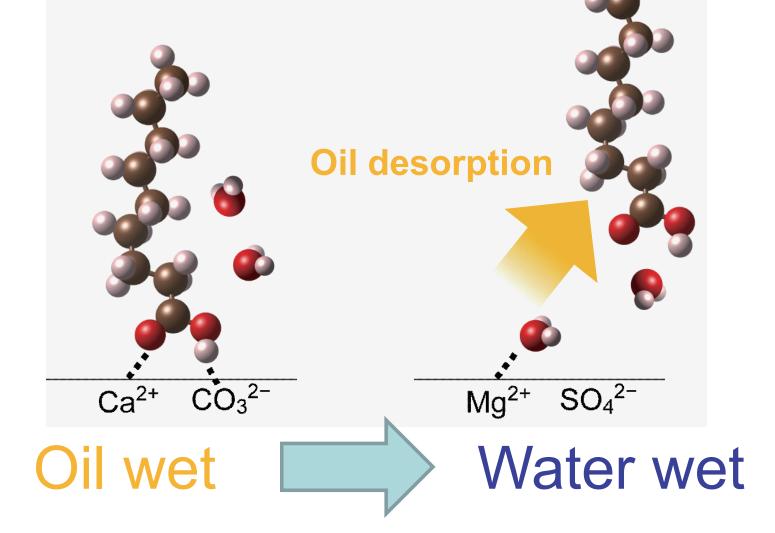
Structure of clay minerals



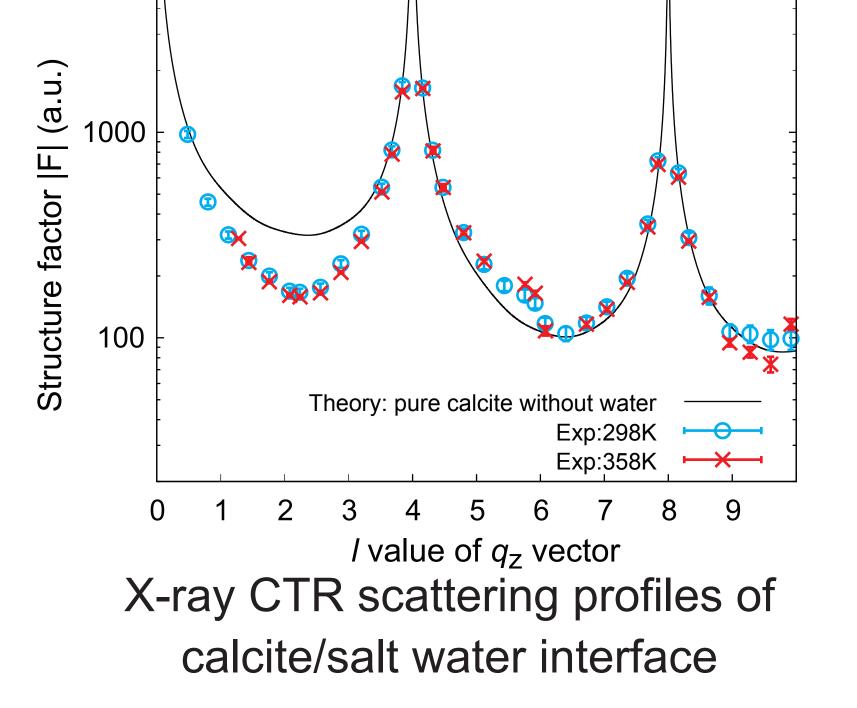
Edges of clay minerals: Extremely reactive in aqueous solution

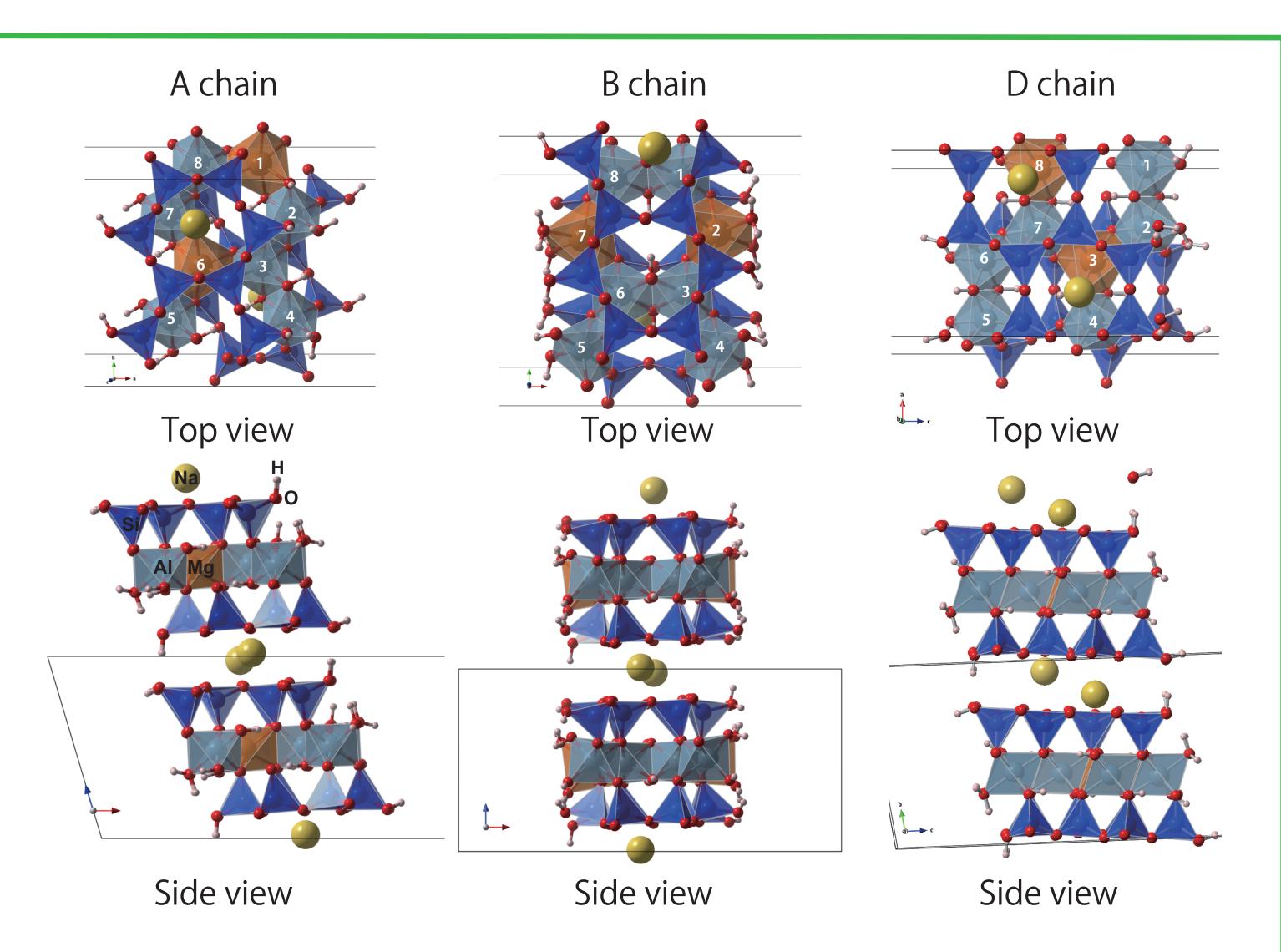
Ion adsorption on edge sites:

Important to use clay minerals as a buffer to retard the radionuclide diffusion from radioactive waste repositories to the outside.



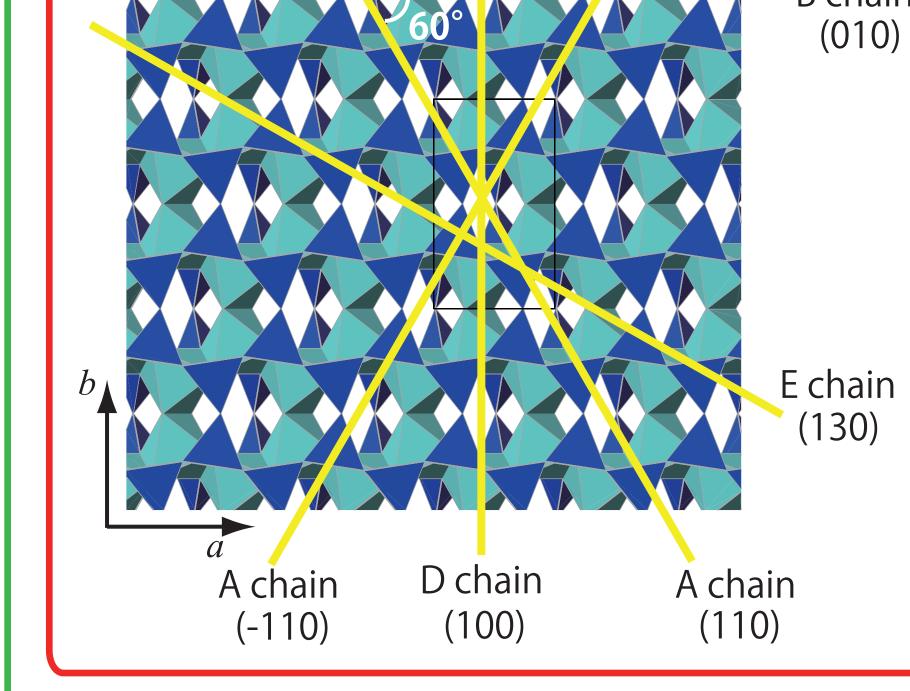
lon substitution (ion switch) induces the desorption of oil molecules





What is a plausible edge plane? Montmorillonite Criteria: White and Zelazny, 1988 B chain

Stable crystal faces are parallel



to one or more continuous chains of strong bonds. A, B chains

(White and Zelazny, 1988) D chain (Churakov, 2006)

2. The smallest unit should consist of one octahedron and one tetrahedron attached for each tetrahedral sheet.

Characterization of edge structures of clay minerals is crucial for developing new functional materials!