Molecular Modeling (2019 – 2024)

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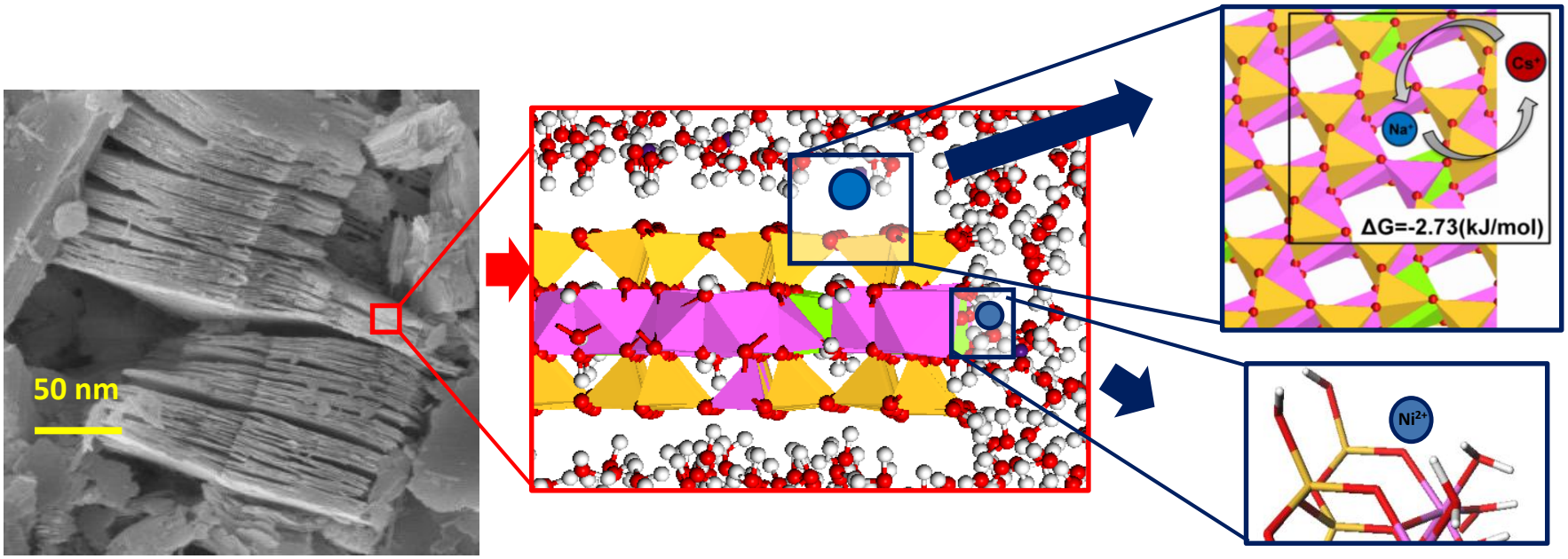

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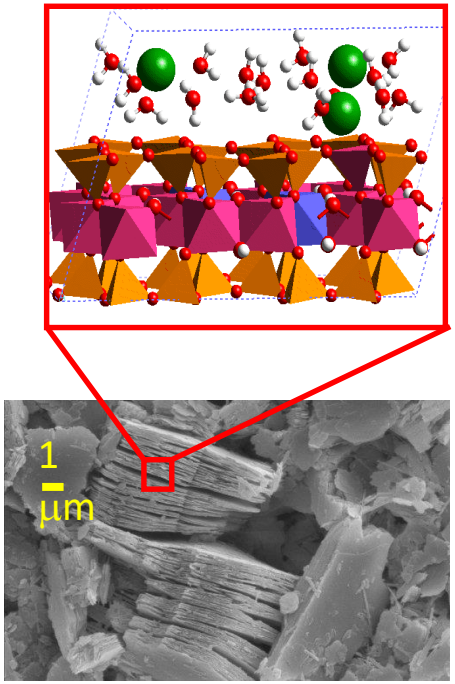
Molecular Modeling at EMN (IMTA) / SUBATECH

- **Molecular Modeling** has been created in 2010 as a new research team within the Radiochemistry Group of SUBATECH in the context of the industrial chair «*Storage and Disposal of Radioactive Waste*» at the Ecole des Mines de Nantes with the focus on the ***computational molecular modeling for radioactive waste disposal applications***
- **Funded by**

ANDRA orano EDF Fondation EDF Science - Enseignement en partenariat avec l'Institut de France

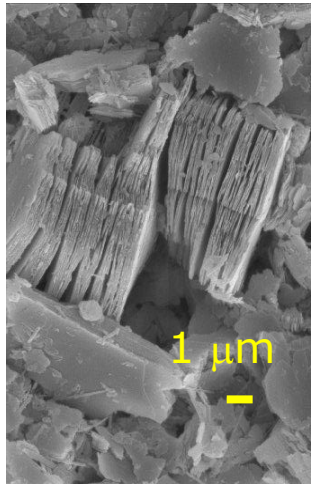


In the general context of ***improving molecular-scale understanding of the interactions between radionuclides, clay and cement materials, and organic molecules***, the specific problems include:

- ✓ Adsorption and mobility of cations and anions in clay environment
- ✓ Effects of clay composition, site substitutions, and edge sites on the adsorption and mobility of radionuclides
- ✓ Effects of organics on the adsorption and mobility of radionuclides in clays
- ✓ Effects of hydrogen bonding and proton transfer on the hydration structure, energetics, dynamics, and chemical reactivity of aqueous cations and anions at clay edges
- ✓ Addressing the same range of problems for cement phases, calcite, quartz, and other materials relevant to radioactive waste disposal

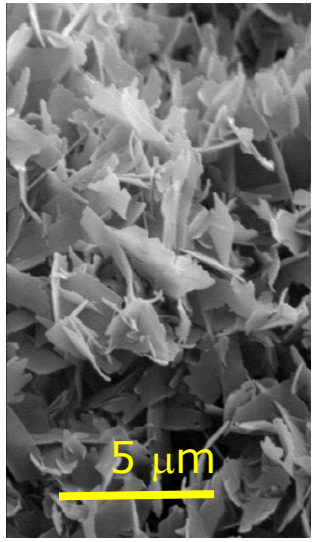
Molecular Modeling - Research Competences and Objectives

Classical and ab-initio atomistic computer simulations of materials for quantitative understanding of the properties and processes of ***clay-related and cement-related systems and their interfaces with fluids*** on the fundamental molecular scale: adsorption and transport of ions (radionuclides); effects of organic molecules; effects of fluid composition; effects of temperature, etc.



Principal Research Directions in the last 5 years (2019-2024):

- ✓ Continuation of the *ClayFF force field* development and parametrization
- ✓ Development of *more realistic models for clayey and cementitious materials* taking into account their natural compositional and structural disorder
- ✓ Quantification of the *effects of specific surface sites* on the adsorption and transport of molecular species in clays and other disordered materials
- ✓ *Role of nano-particle edges* in the clay and cement modeling
- ✓ Quantification of the *effects of molecular gases (H_2, CO_2, CH_4,..)* on the adsorption and transport of radionuclides clay and cement materials
- ✓ *Effects of organic matter* on the complexation and aggregation of ions in clay and cement materials
- ✓ *Effects of temperature and other thermodynamic conditions* on the above processes



Classical Molecular Dynamics (MD) Simulations

- Classical simulations calculate energy and forces between atoms based on a **force field** that is a set of parameters describing atomic interactions
- The **length-** and **time- scales** of classical MD can reach **~1 μm** and **~1 μs**

Numerically solve Newtonian equation of motion for *N* interacting particles:

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\,\Delta t + \tfrac{1}{2}\,\mathbf{a}_i(t)\,\Delta t^2 \quad ; \qquad \Delta t \sim 1 \text{ fs} = 10^{-15} \text{ s}$$

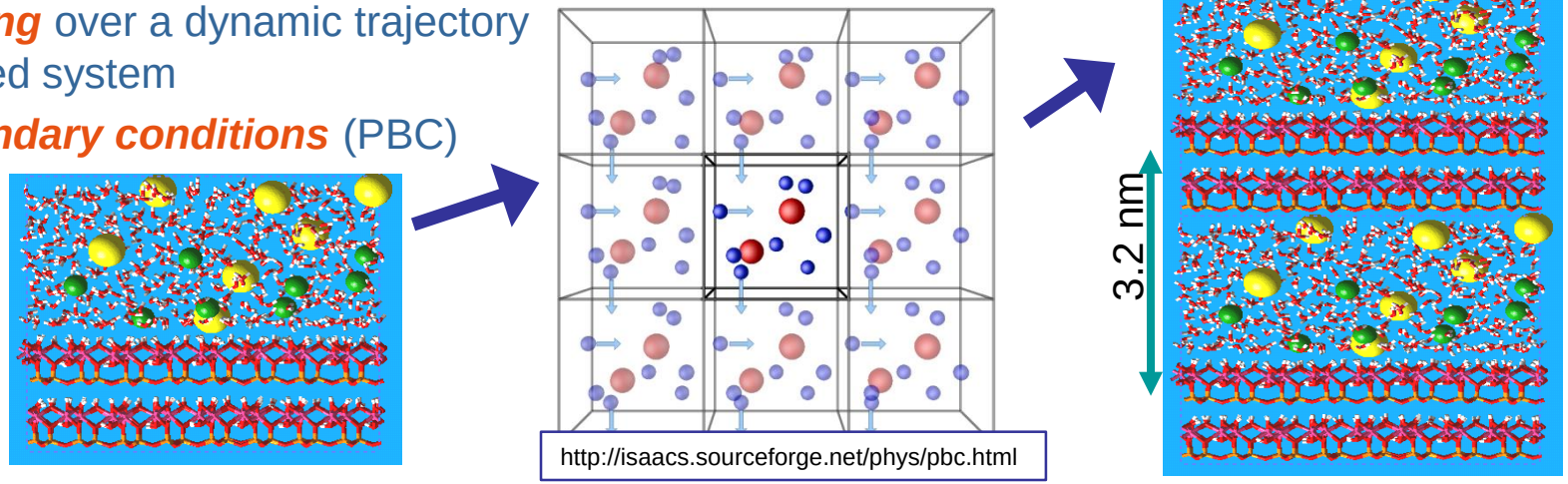
$$\mathbf{a}_i = \mathbf{F}_i/m = [\, -\partial U(\mathbf{r}_1, \mathbf{r}_{2,\ldots}\, \mathbf{r}_N) / \partial \mathbf{r}_i \,] / m \quad ; \qquad i = 1, 2, \ldots, N \quad (N \sim 10^3 - 10^6 \text{ atoms})$$

$$U = \Sigma\Sigma U_{ij} = \Sigma\Sigma(A_{ij}/r_{ij}^{12} - B_{ij}/r_{ij}^{6} + q_i q_j /e_0 r_{ij}) + \Sigma\, \tfrac{1}{2}k_b\,(r_{ij} - r_0)^2 + \Sigma\, \tfrac{1}{2}k_\theta\,(\theta_{ij} - \theta_0)^2$$

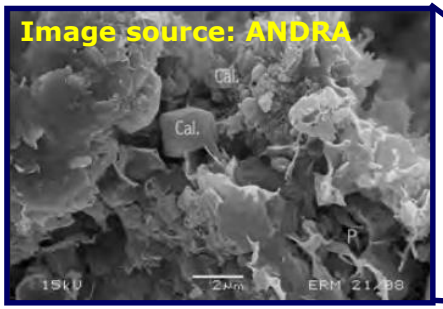
Short-range repulsion | v-d-Waals | Coulombic | bond stretching | bond bending

Time averaging over a dynamic trajectory of the simulated system

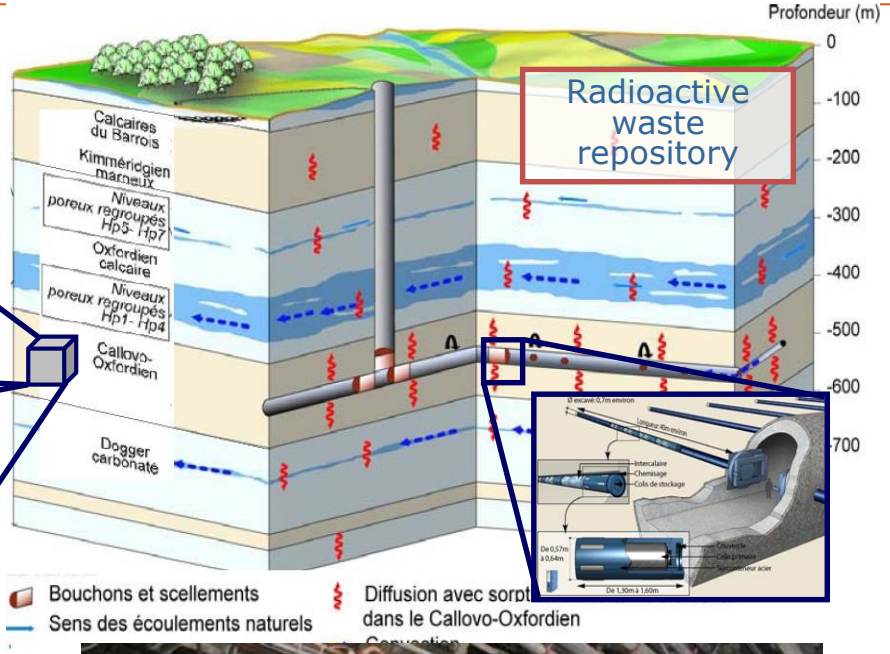
Periodic boundary conditions (PBC)



Molecular-Scale Understanding of the Adsorption and Transport of Radionuclides in Cox Clay Formations



- 41% clay (illite, smectite, and interstratified I/S)
- 31% calcite
- 25% quartz and feldspar
- 3% other minerals
- ~1% organic matter



Simulating clay and cement is non-trivial

- Variable composition, low symmetry, complex crystal structures
- Incompletely and poorly characterized, occur as very fine-grained material
- **Availability of empirical force-fields for realistic molecular modeling**

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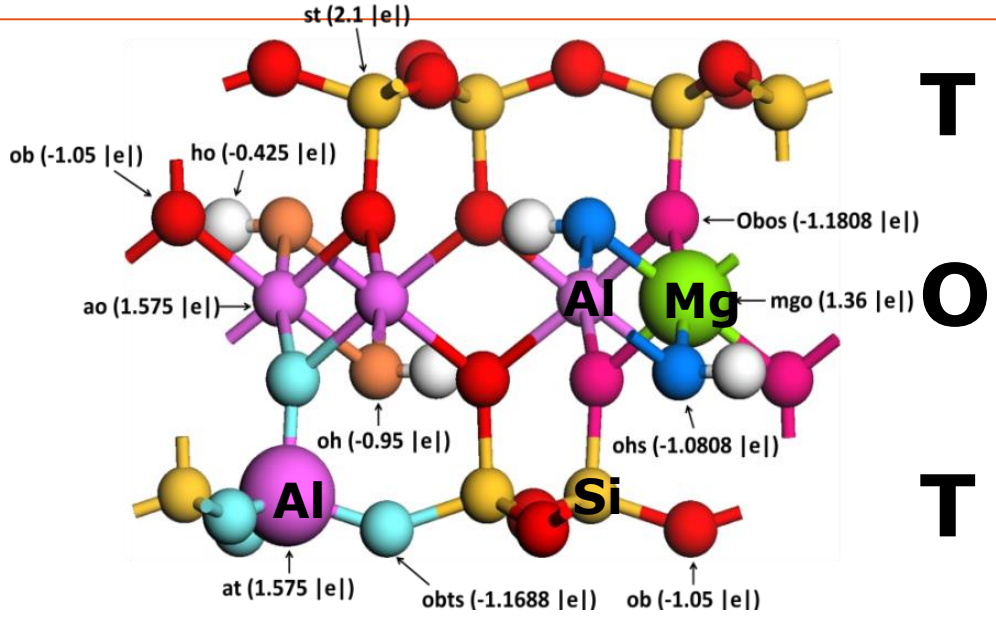
ClayFF Construction and Parametrization

1. **No explicit bonds – quasi-ionic**
2. **LJ parameters for all oxygen atoms are assumed to be equal to Ow for SPC water**

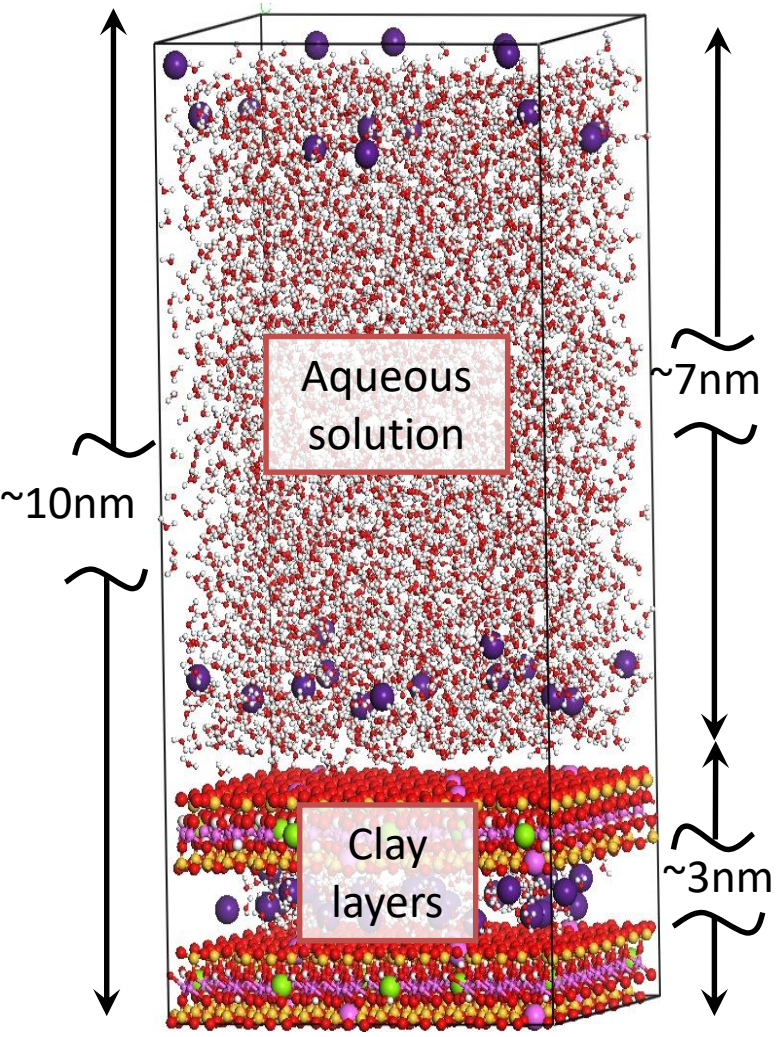
Both assumptions are great simplifications of reality, but they seem to work quite well



- ***Accurate determinations of partial charges*** are required to represent charge distributions of interlayer and external surfaces where electrostatic forces control sorption and transport processes
- Atomic charges derived from ***DFT calculations*** for cluster and periodic models of ***simple oxide and hydroxide phases:*** $Mg(OH)_2$, $Al(OH)_3$, SiO_2, kaolinite…
- Allows for ***charge delocalization*** among coordinating oxygens for substitutions

ClayFF: Cygan, Liang, Kalinichev, *J. Phys. Chem. B*, **108** 1255-1266 (2004)
Cygan, Greathouse, Kalinichev, *J. Phys. Chem. C*, **125** 17573-17589 (2021)

MD Modeling of Clay-Solution Interfaces



Classical Newtonian dynamics

- N_{tot} ~ 3,000 – 10,000 atoms
- N_{H2O} ~ 0 – 1,000 molecules
- *ClayFF* force field (Cygan et al., 2004)
- $a \times b \times c$ ~ $3 \times 3 \times 10$ nm^3
- Periodic boundary conditions
- *NVT*- or *NPT*-ensemble T=300K; P =1 bar
- t ~ 200 - 1,000 ps
- Δt = 0.5-1.0 fs

Solution structure:

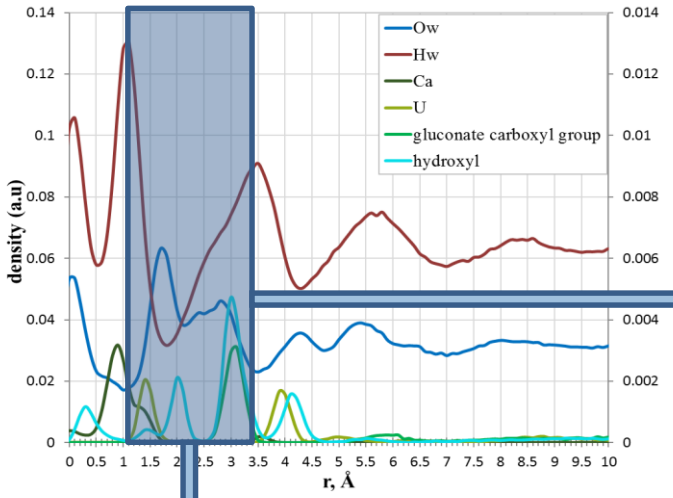
- ✓ Atomic density profiles ($\perp$)
- ✓ Atomic density surface distributions ($\parallel$)
- ✓ Topology of the interfacial H-bond network

Dynamics:

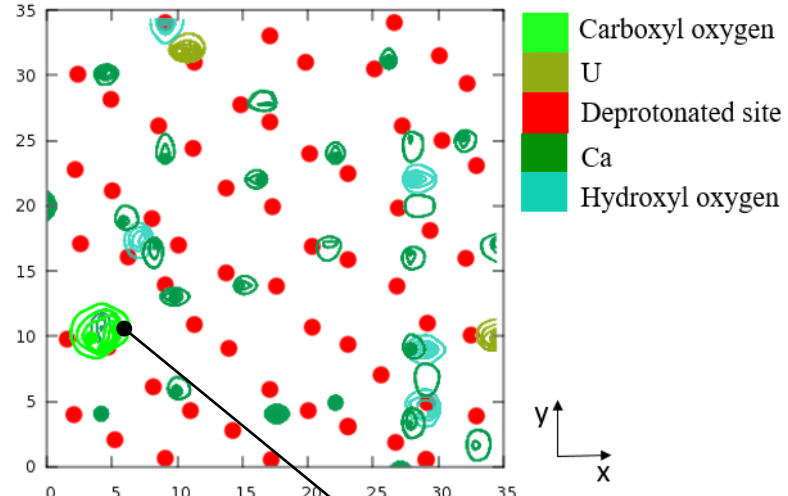
- ✓ Diffusion coefficients (longer time scale)
- ✓ Spectra of vibrational and rotational dynamics (shorter time scale)

Uranyl / Gluconate Solutions on the C-S-H surfaces

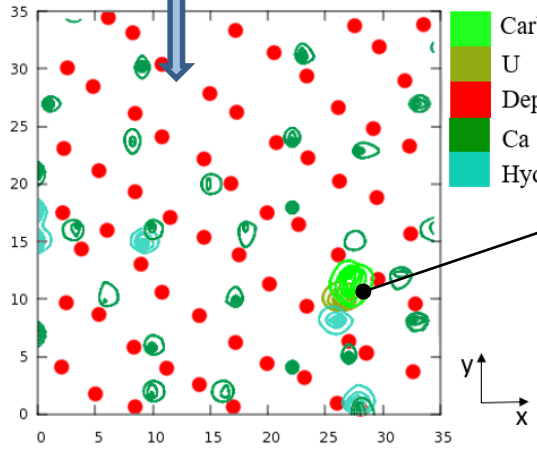
Atomic density profiles normal to the C-S-H-1.4 surface for the solution with UO_2^{2+} and gluconate

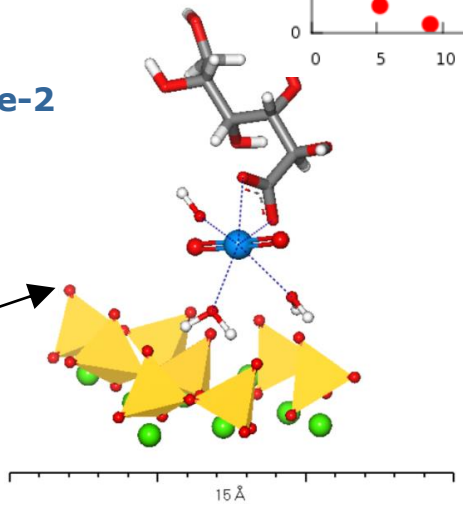


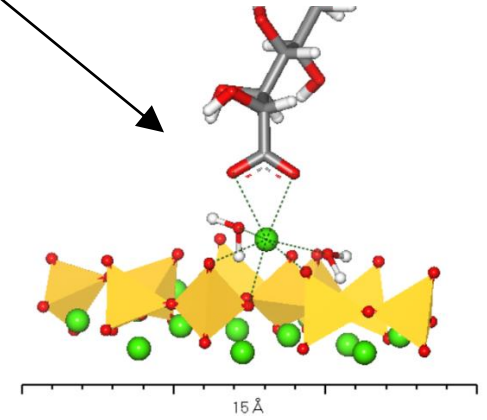
Distribution of ions on the C-S-H-1.4 surface-1



Distribution of ions on the C-S-H-1.4 surface-2

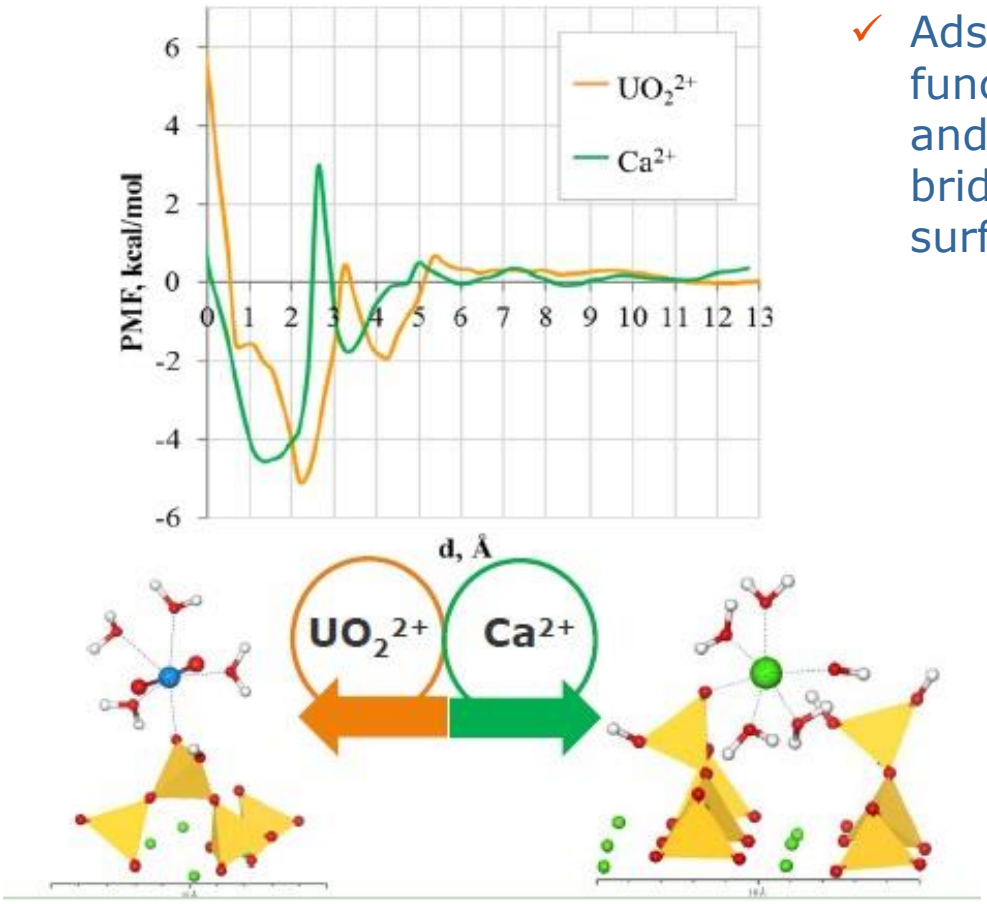






I.Androniuk, A.G.Kalinichev (2020) *Appl. Geochem.*, **113**, 104496

Competition of UO_2^{2+} and Ca^{2+} for Adsorption Sites

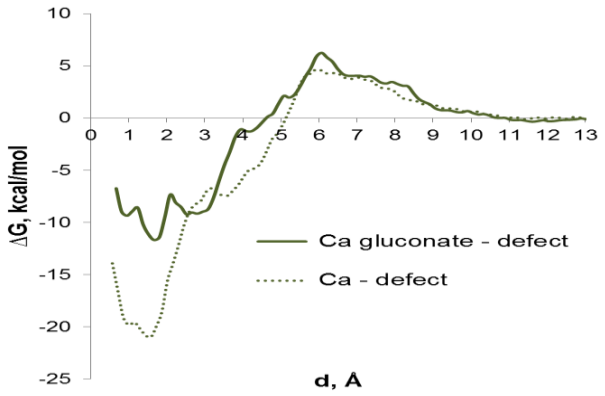


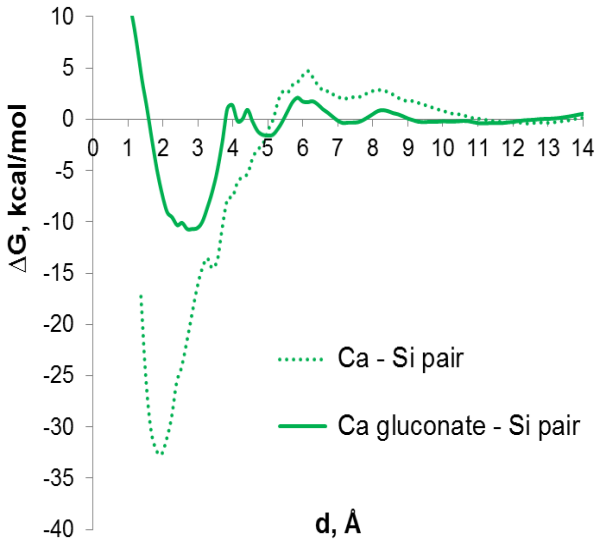
- ✓ Adsorption free energy (PMF) as a function of distance between UO_2^{2+}, Ca^{2+} and deprotonated silanol group of the bridging Si tetrahedra on the C-S-H surface at C/S = 0.83

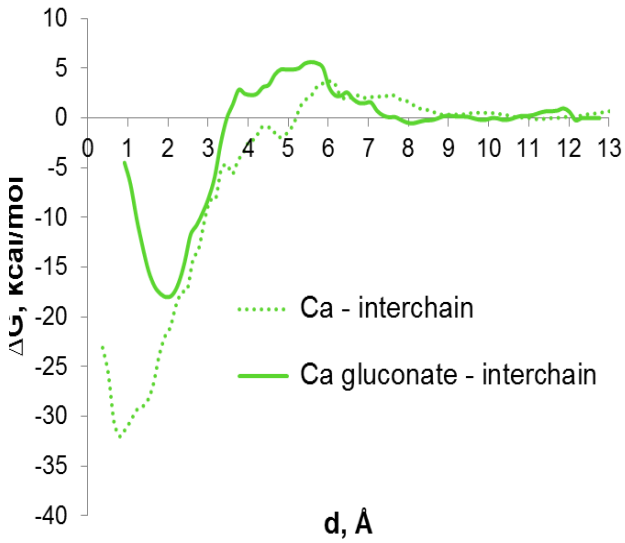
- ✓ High energy barrier between the inner-sphere (IS) and outer-sphere (OS) surface complexes
- ✓ Approximately the same depth of the potential wells for both IS and OS
- ✓ Ion exchange and competition for the same surface sites are very likely

I.Androniuk, C.Landesman, P.Henocq, A.G.Kalinichev (2017) *Phys. Chem. Earth A/B/C,* **99**, 194-203
I.Androniuk, A.G.Kalinichev (2020) *Appl. Geochem.*, **113**, 104496
P.Henocq, C.Landesman, I.Androniuk, A.G.Kalinichev (2024) *Cement and Concrete Research*, in prep.

Effect of Gluconate on Ion Binding to C-S-H Surface







- ✓ The binding of Ca^{2+} to the C-S-H surface becomes much weaker and potentially may result in a higher probability of substitution for a competing solution cation (e.g., Na^{+} or $UO_2(OH)_3^{-}$)
- ✓ Effect of gluconate is the same for all the sorption sites studied.
- ✓ Even though the adsorption energy decreases, complexation between Ca-gluconate and C-S-H surface remains stable.

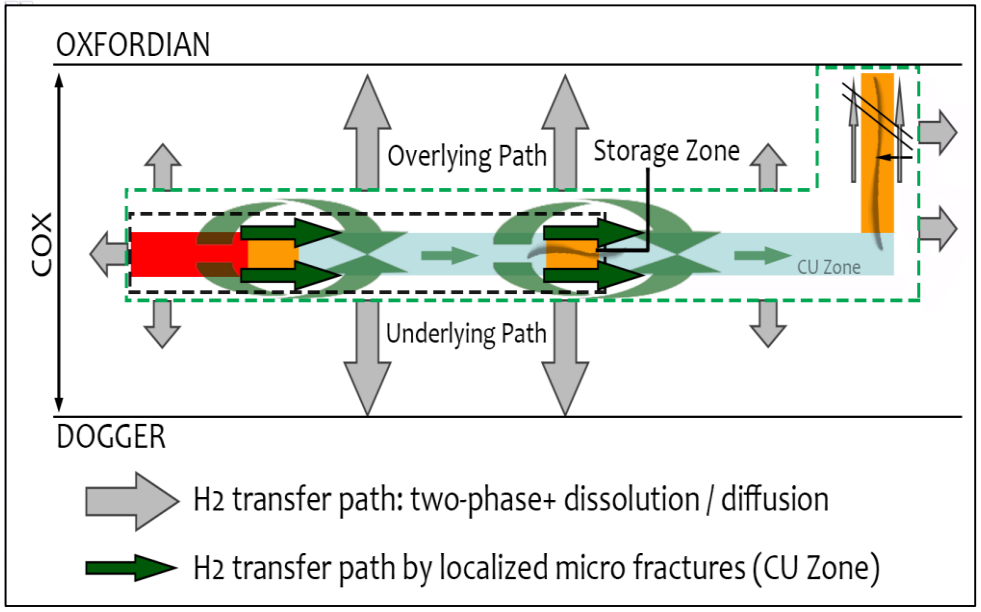
I.Androniuk, A.G.Kalinichev (2020) *Appl. Geochem.*, **113**, 104496

P.Henocq, C.Landesman, I.Androniuk, A.G.Kalinichev (2024) *Cement and Concrete Research*, in prep.

Gas Formation under Waste Storage Conditions

PhD thesis of Pinar CITLI (February 2024)

Anaerobic corrosion of metals	Degradation of organic matter	Radiolysis of water due to radioactive decay
H_2	CH_4	H_2
	CO_2	O_2
		CO_2
		CH_4



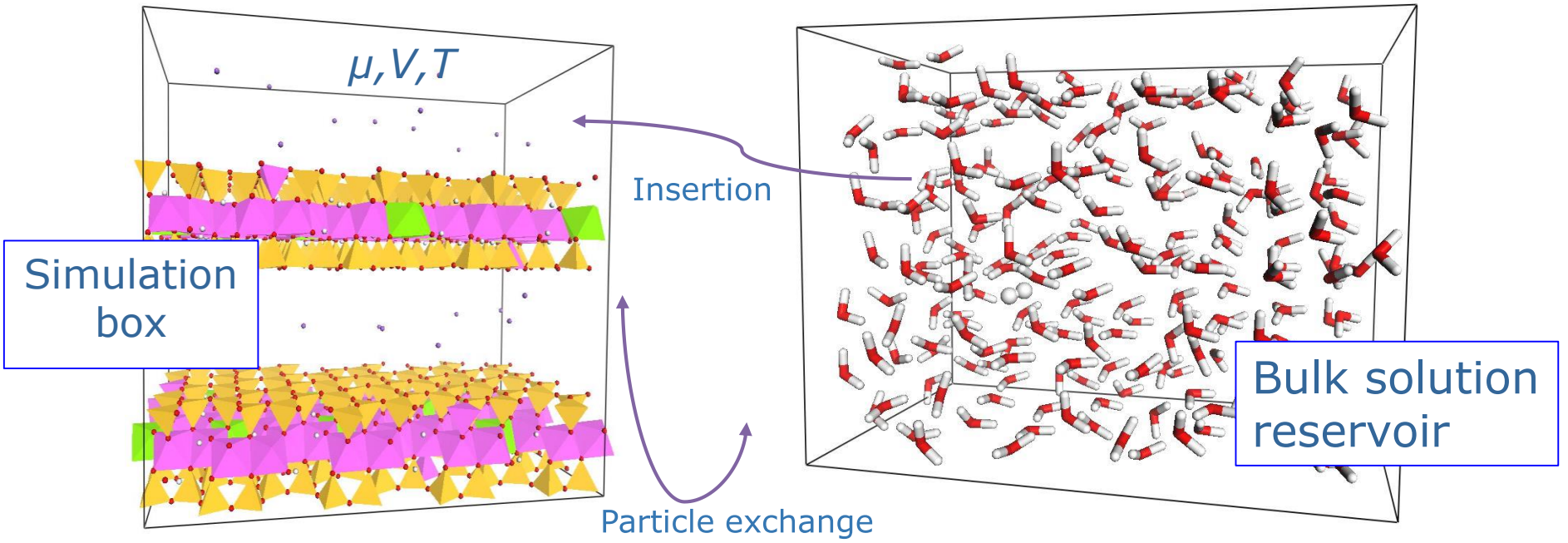
Gas accumulation → Gas pressure build-up → Over pressure → Fracture of surrounding clay rock

- ✓ Dissolution in water and diffusion
- ✓ Two-phase water flow
- ✓ Transfer along micro fractures
- ✓ Transfer along fractures

GCMC simulations of H_2 Adsorption in Clay

PhD thesis of Pinar CITLI (February 2024)

- ✓ Grand Canonical Monte Carlo (GCMC) simulations of H_2/H_2O binary mixtures
- ✓ T = 298, 323 and 363 K ; P = up to 120 bar, 1000 bar and 10,000 bar

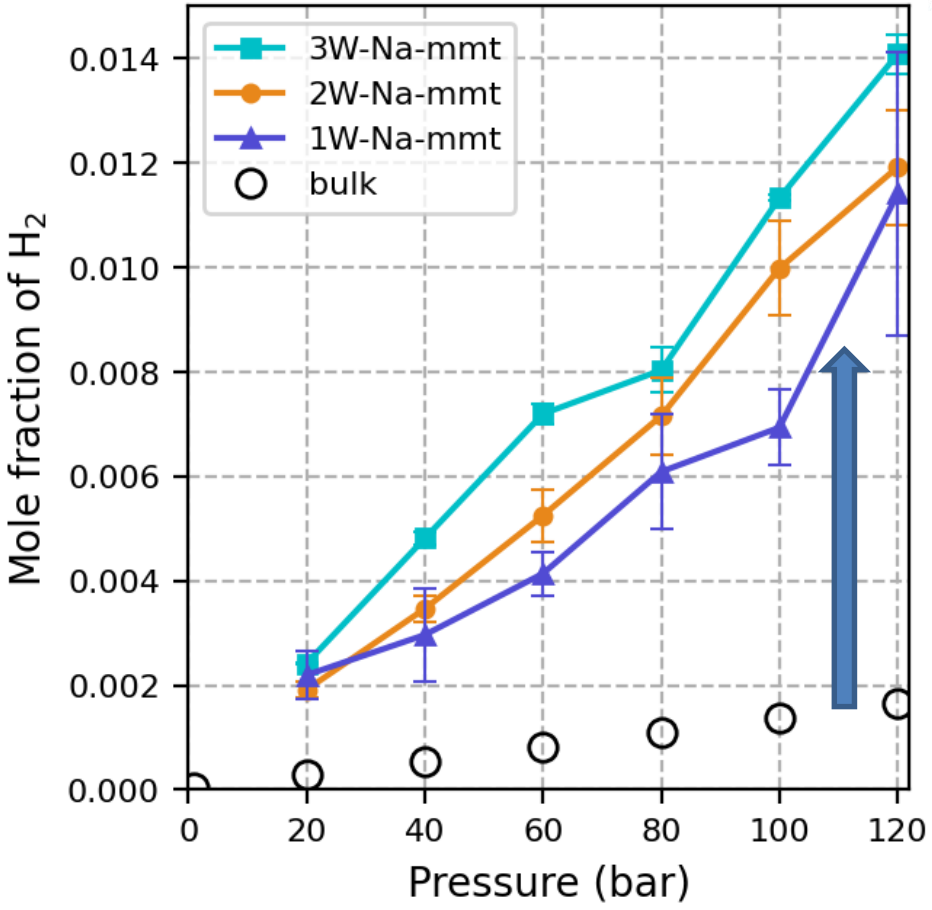


- ✓ Solubility of H_2 in the clay interlayers
- ✓ Effect of pore size and hydration level
- ✓ Effect of interlayer cation

- ✓ Effect of temperature
- ✓ Effect of pressure
- ✓ Comparison of simulations results with experimental data

Oversolubility of H_2 in the interlayers

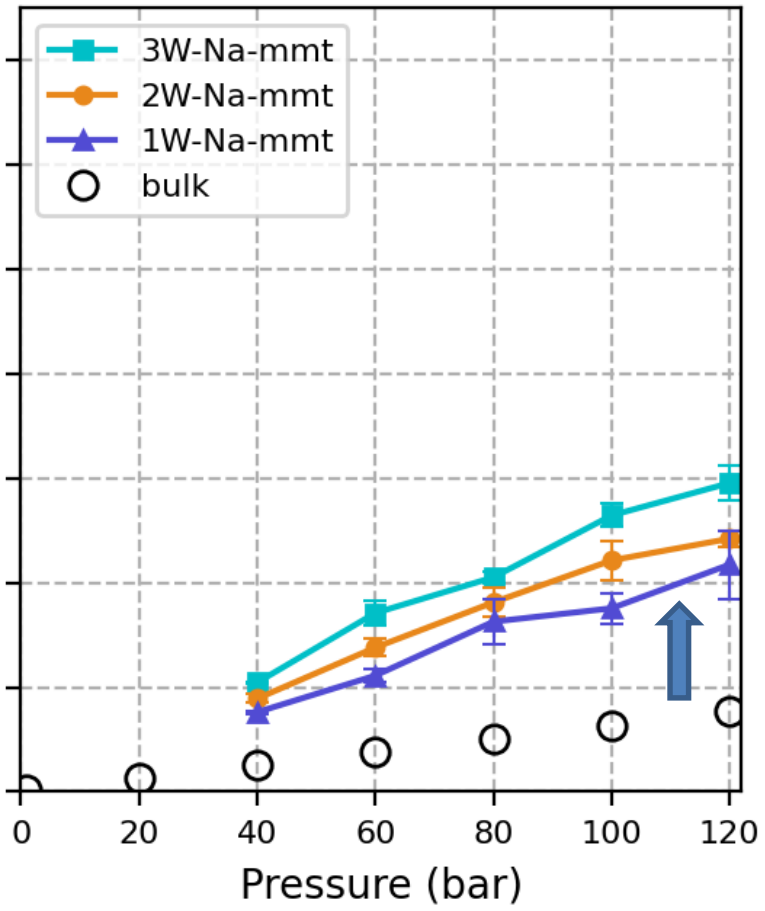
298 K



7 to 8 times greater solubility than in bulk

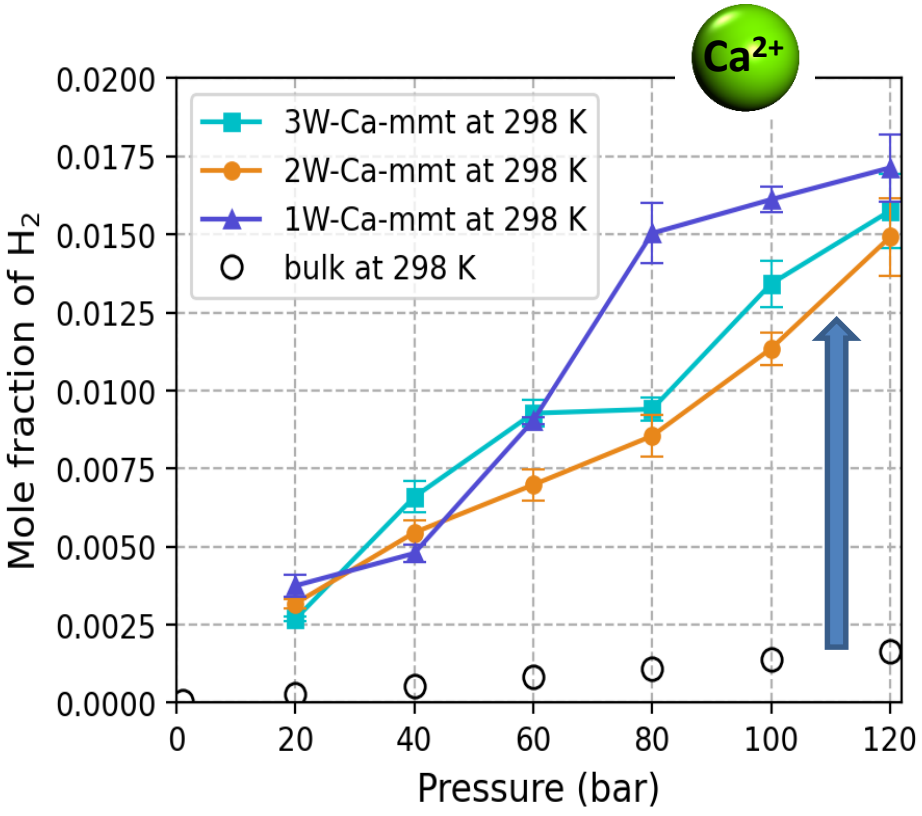
Na+

323 K

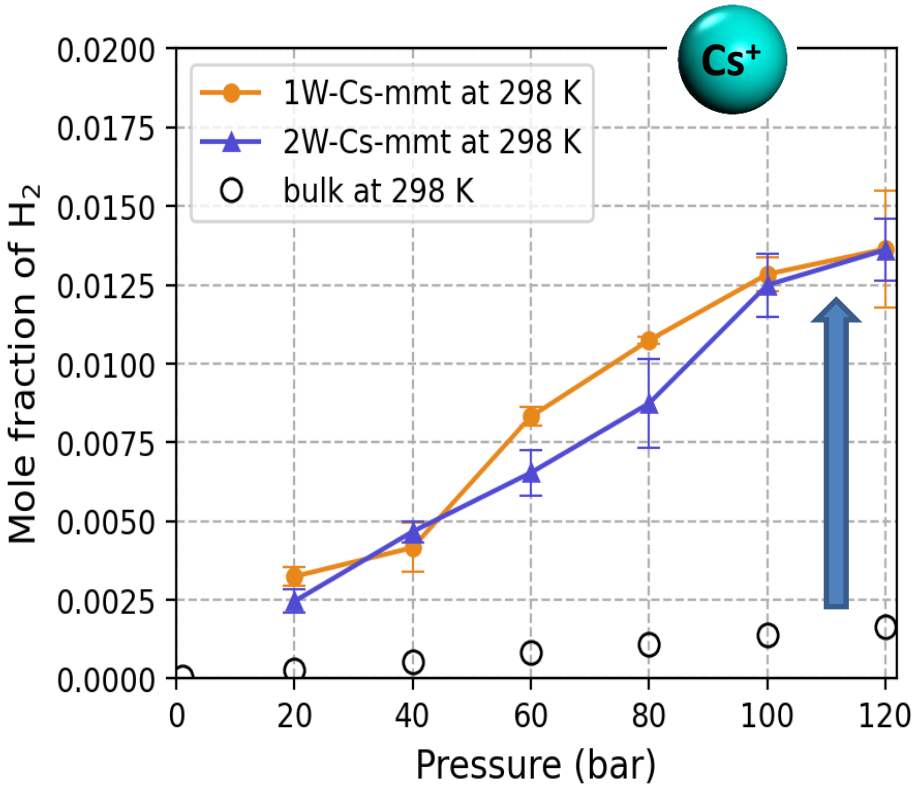


2 to 4 times greater solubility than in bulk

Oversolubility of H_2 in the interlayers



Up to 9 times greater solubility than in the bulk

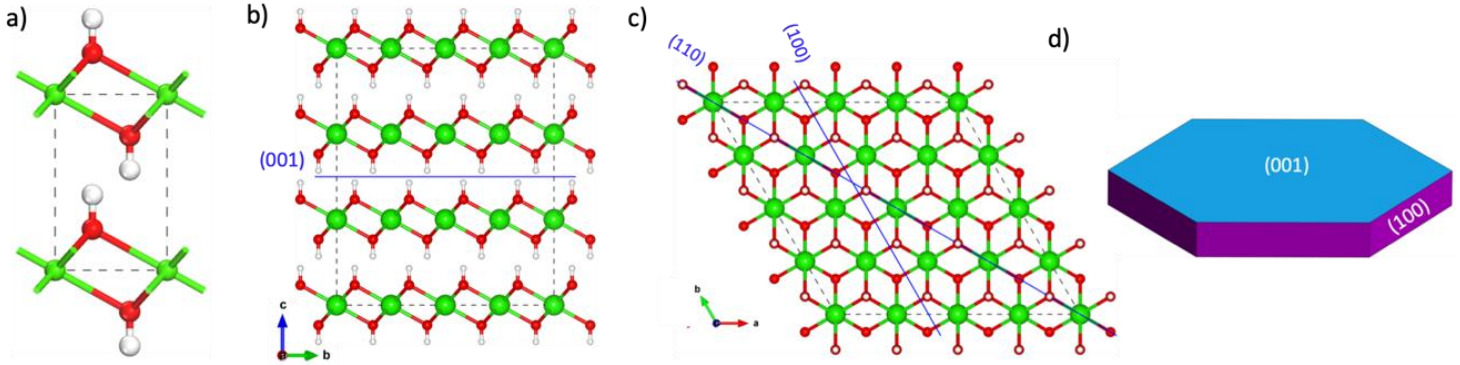


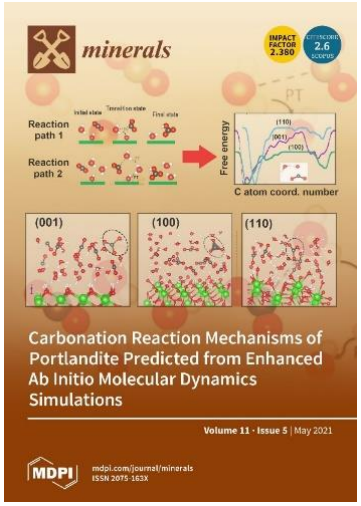
8 times greater solubility than in the bulk

P.Citli, A.G.Kalinichev (2024) Grand Canonical Monte Carlo simulations of hydrogen adsorption in the interlayers of hydrated montmorillonite. *Applied Clay Science*, (submitted).

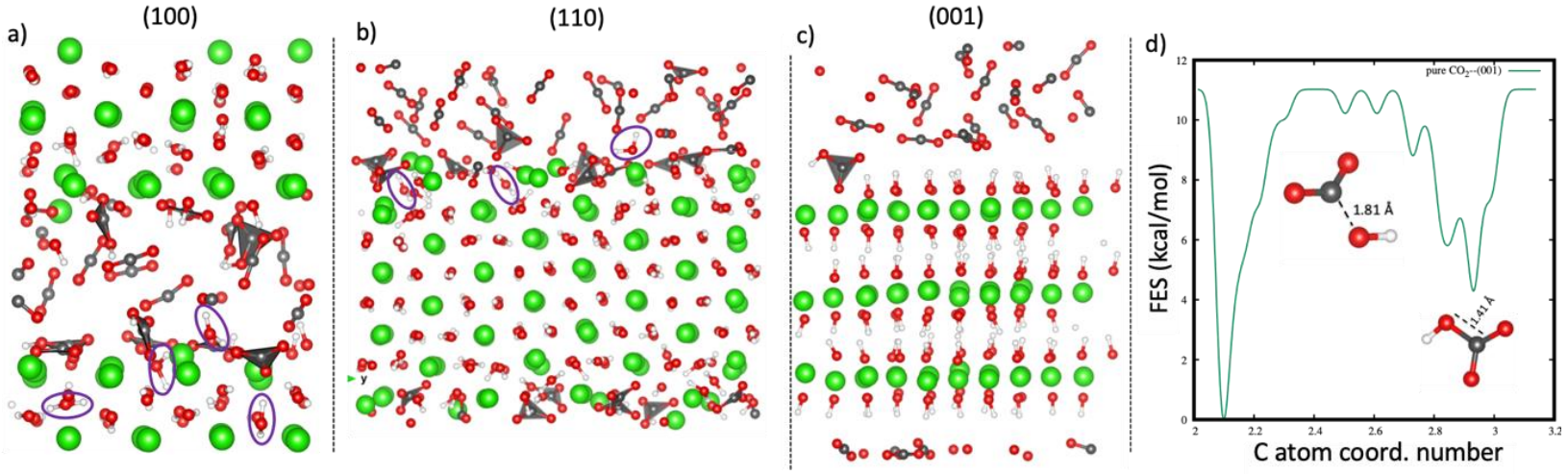
Reactivity of CO_2 with Portlandite Surfaces – Ab Initio MD

$$Ca(OH)_2 + CO_2 \longrightarrow CaCO_3 + H_2O$$



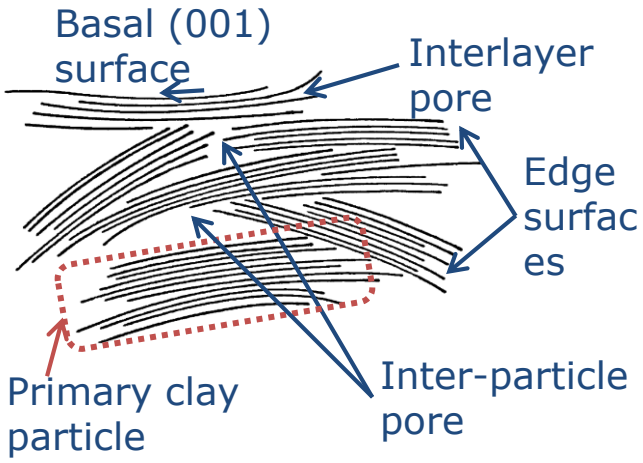


S.Mutisya, A.G.Kalinichev, *Minerals,* **11**, 509 (2021)



ClayFF Development - Modeling of Particle Edges

Aggregate of clay particles



- Basal (001) surfaces and interlayers are extensively studied; their properties are reasonably well known
- Clay edges have received much less attention yet
- Ab initio (quantum) MD is a direct answer, but it is very expensive computationally
- AIMD ⇒ ~n×100 atoms; ~15×15×15Å^3; t ~10-50 ps

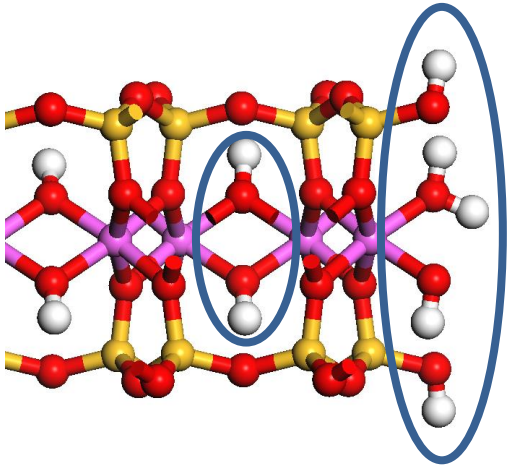
S.V.Churakov, *Geochim. Cosmochim. Acta*, **71**, 1130-1144 (2007)
X. Liu et al., *Geochim. Cosmochim. Acta* (2012, 2013, 2014, 2015)
S. Tazi et al., *Geochim. Cosmochim. Acta*, **94** 1-11 (2012)

ClayFF Parametrization for Clay Edges

New special ClayFF bending terms for Mg-O-H, Al-O-H, and Si-O-H

$$U_{\text{ClayFF-MOH}} = U_{\text{ClayFF-orig}} + U_{\text{M-O-H}} = U_{\text{ClayFF-orig}} + k\,(\theta-\theta_0)^2$$

k and θ_0 have to minimize the differences between DFT and ClayFF-MOH results



Pouvreau, Greathouse, Cygan, Kalinichev, *J.Phys.Chem.C*, **121**, 14757-14771; 2019, **123**, 11628–11638

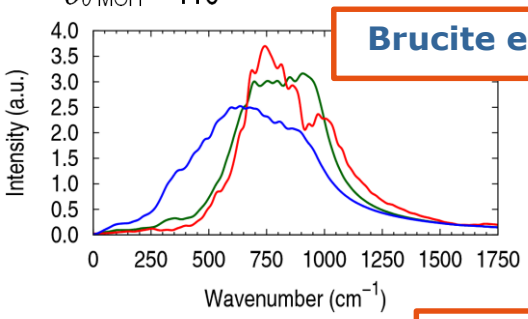
ClayFF: O-H Librational (M-O-H Bending) Spectra

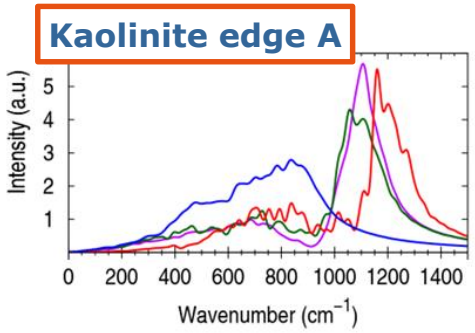
DFT
CLAYFF-orig
CLAYFF-MOH:
k_{MgOH} = 6 kcal·mol^{-1}·rad^{-2}
k_{AlOH} = k_{SiOH} 15 kcal·mol^{-1}·rad^{-2}
$\theta_{0\ MOH}$ = 100°
$\theta_{0\ MOH}$ = 110°

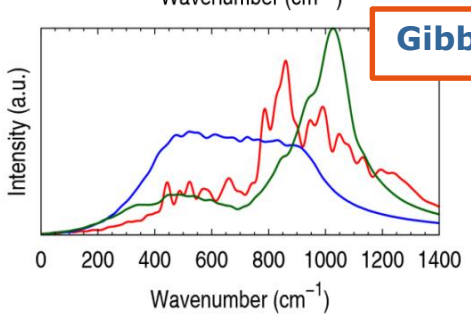
Fourier Transform of the velocity autocorrelation function:

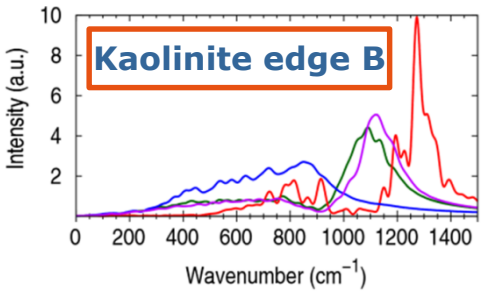
$$P(\nu) = \int \langle \dot{\boldsymbol{r}}(\tau) \cdot \dot{\boldsymbol{r}}(t+\tau) \rangle_\tau \, e^{-i\omega t} dt$$

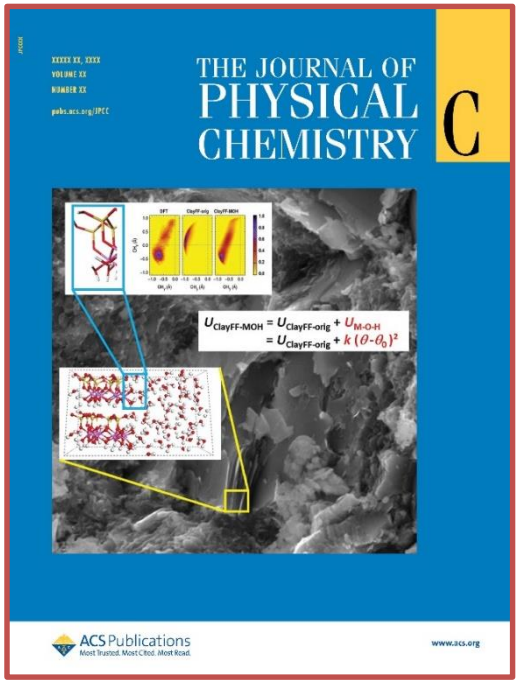
Velocity of the H atoms of O-H groups → $\bar{\nu}$ < 1500 cm^{-1}: O-H libration











- ✓ Spectra shifted of 250 to 600 cm^{-1} and narrowed
- ✓ Kaolinite: as expected not much difference between θ_0=100° and θ_0=110°

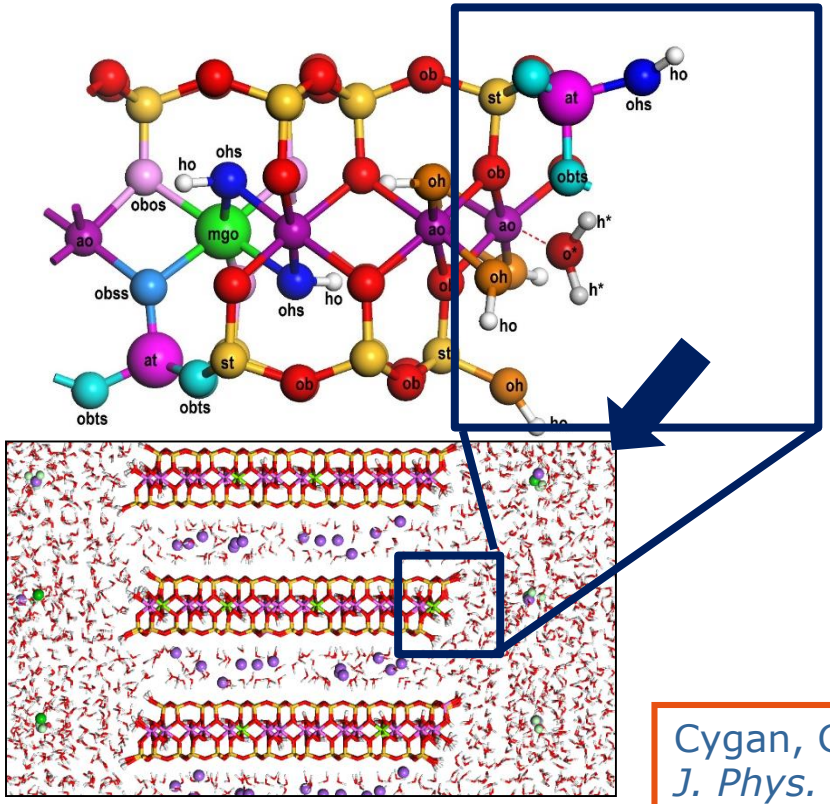
M.Pouvreau, J.A.Greathouse, R.T.Cygan, A.G.Kalinichev, *J.Phys.Chem.C*, 2019, **123**, 11628–11638

ClayFF Development - Modeling of Particle Edges

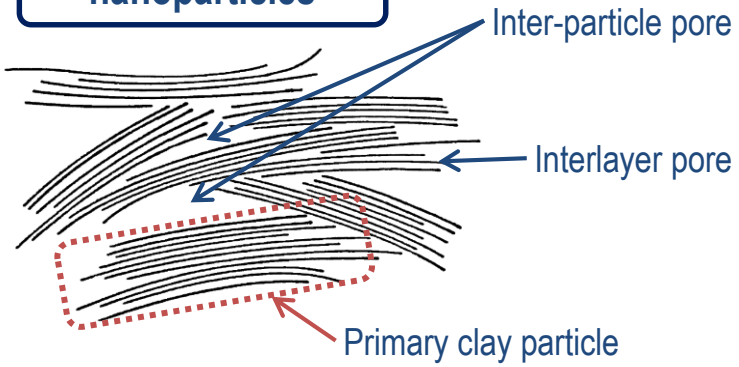
Advances in Clayff Molecular Simulation of Layered and Nanoporous Materials and Their Aqueous Interfaces

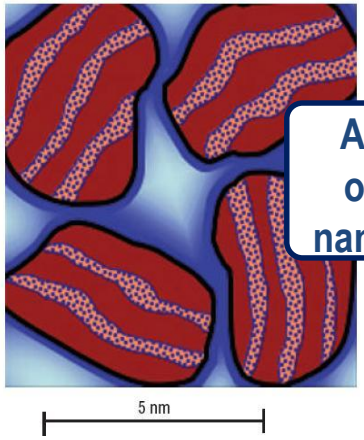
Randall T. Cygan, Jeffery A. Greathouse,* and Andrey G. Kalinichev

Cite This: *J. Phys. Chem. C* 2021, 125, 17573–17589 Read Online

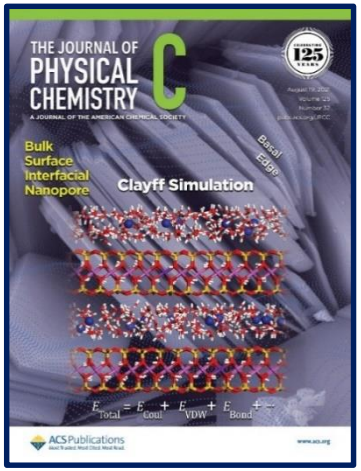


Aggregate of clay nanoparticles





Aggregate of cement nanoparticles



Cygan, Greathouse, Kalinichev (2021)
J. Phys. Chem. C, **125** 17573-17589

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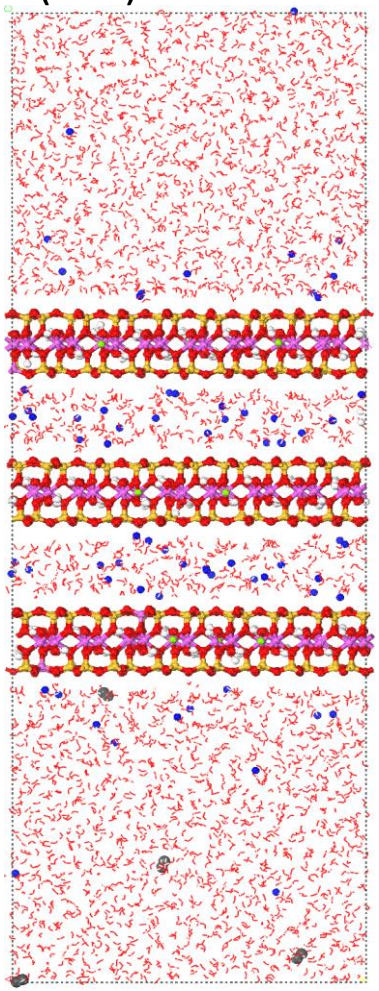
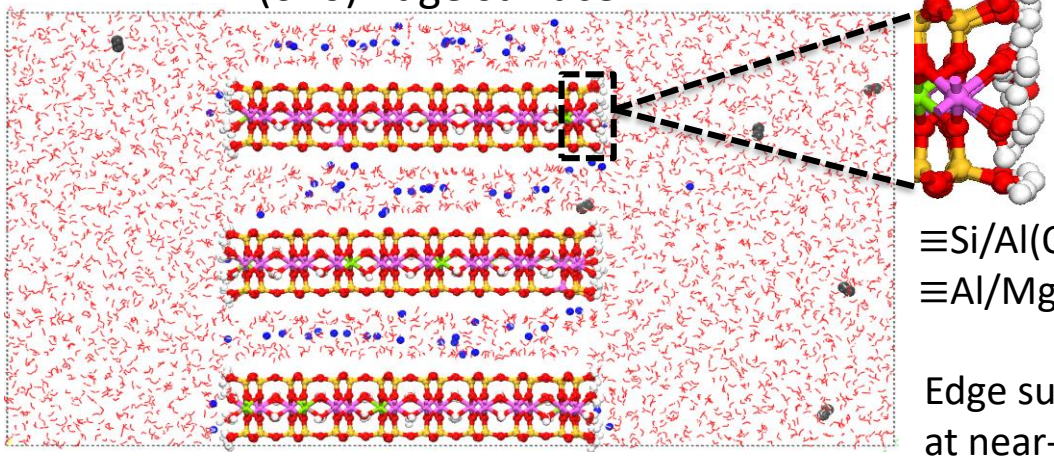
Montmorillonite Clay Nanoparticle Edge Surfaces

(001) Basal surface



(010) Edge surface

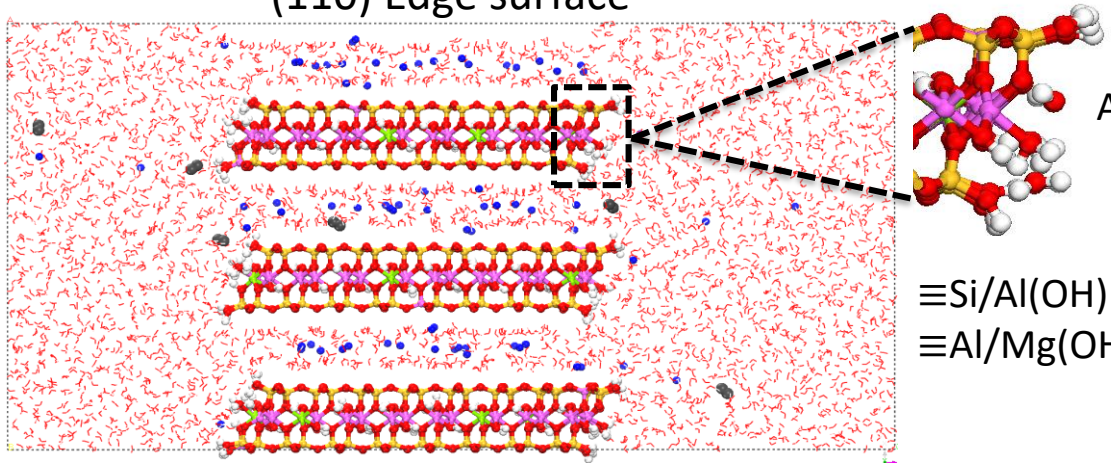


B chains

≡Si/Al(OH) and
≡Al/Mg(OH_2)(OH) sites

Edge surface protonation at near-neutral pH

(110) Edge surface

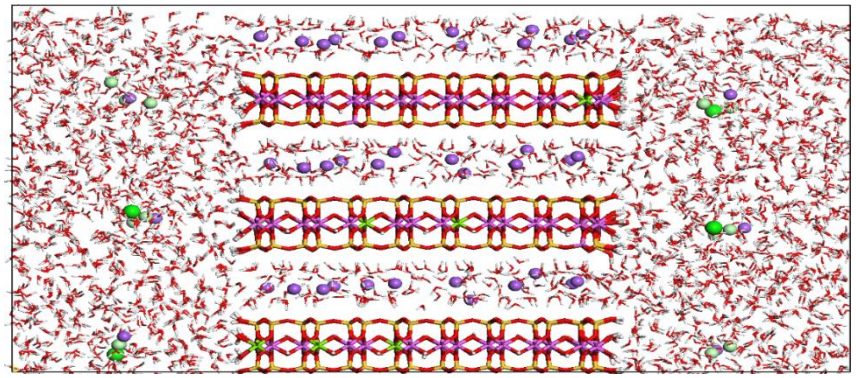


AC chains

≡Si/Al(OH) and
≡Al/Mg(OH_2) sites

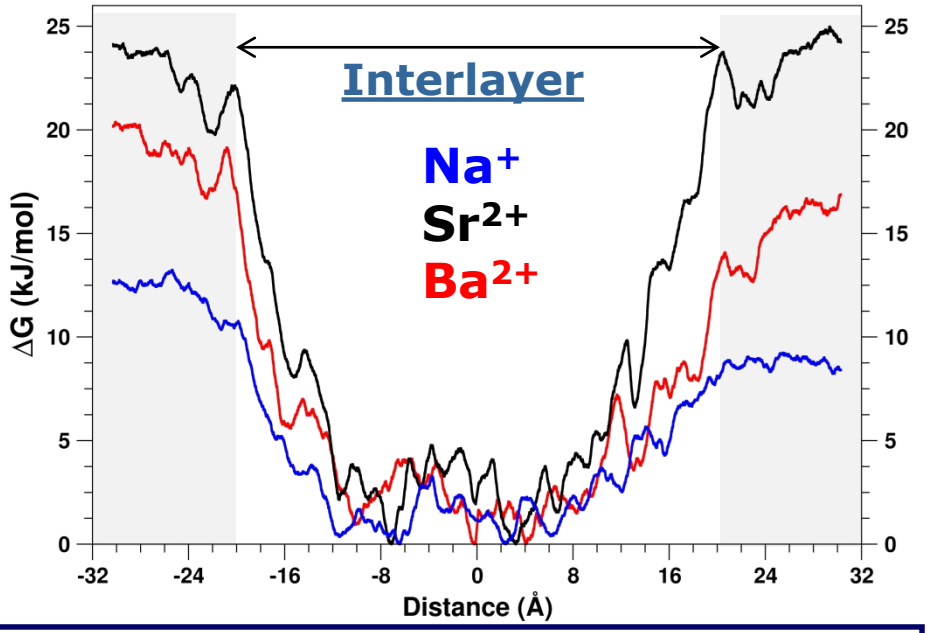
B.F.Ngouana-Wakou et al., *J.Phys.Chem.C*, 2024, in prep.

Interlayer *vs* Edge Adsorption of NORM in Clay



- ✓ All cations are more stable in the interlayer compared to the interface
- ✓ The associated average free energy gain are as follows :
  - **~10 kJ/mol for Na^+**
  - **~25 kJ/mol for Sr^{2+}**
  - **~19 kJ/mol for Ba^{2+}**

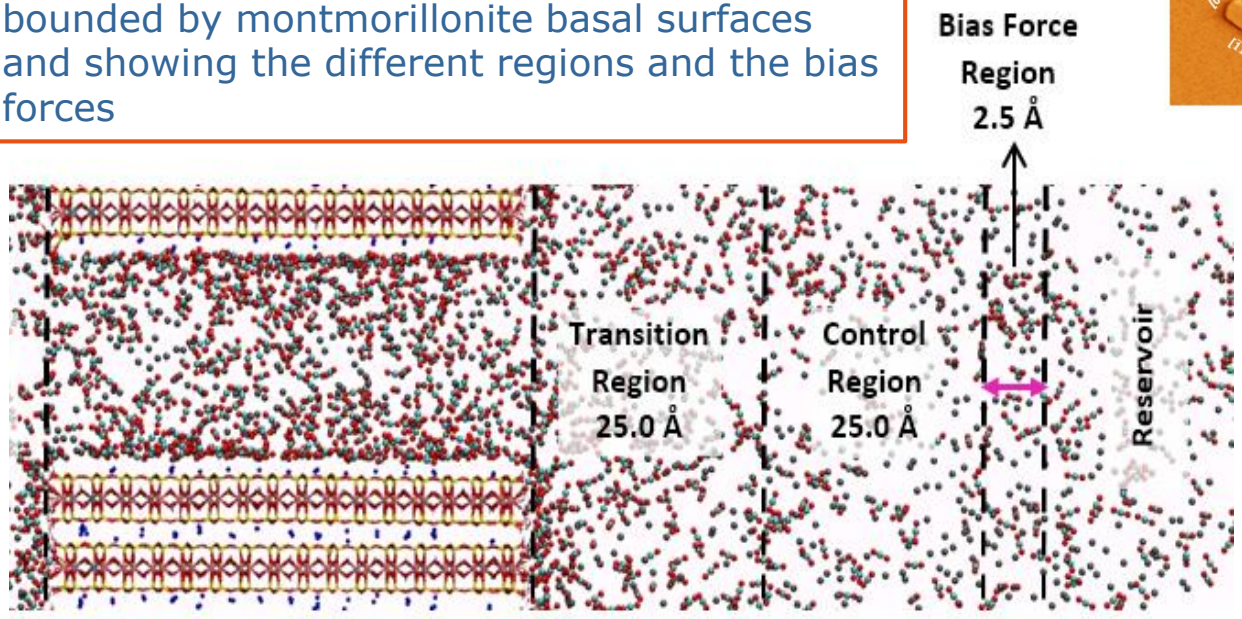
- ✓ The energy gain when Na^+ enters the interlayer region is almost doubled for Sr^{2+} and Ba^{2+}: 1 Sr^{2+}/Ba^{2+} for 2 Na^+ ions
- ✓ This is consistent with our statistical analyses showing that ~70% of Sr^{2+}/Ba^{2+} initially present in the interfacial region migrate in the interlayers during the simulations
- ✓ There are noticeable energy barriers at the (010) edge for Sr^{2+}/Ba^{2+} to enter the MMT interlayers

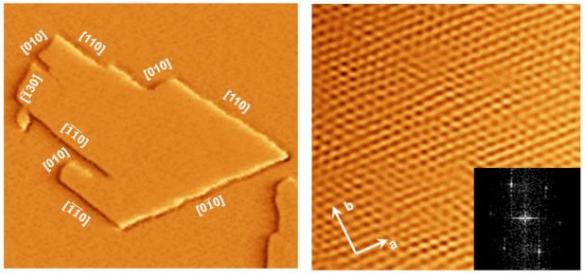


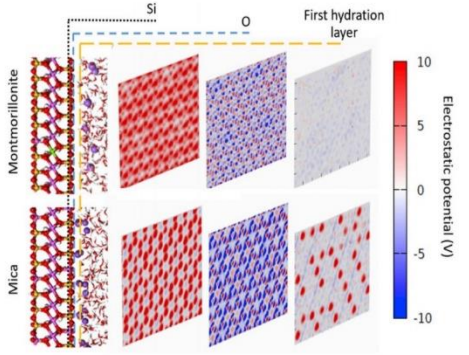
B.F.Ngouana-Wakou et al., *J.Phys.Chem.C*, 2024, in prep.

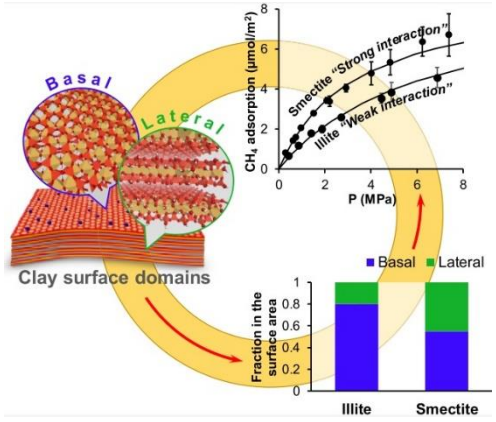
CO_2 and CH_4 Gases in Clay Nanoparticles

Simulation cells used in the constant reservoir composition molecular dynamics (CRC-MD) calculations of CO_2/CH_4 partitioning into pores bounded by montmorillonite basal surfaces and showing the different regions and the bias forces









N.Loganathan et al. (2019) *Phys.Chem.-Chem.Phys*, **21**, 6917-6924

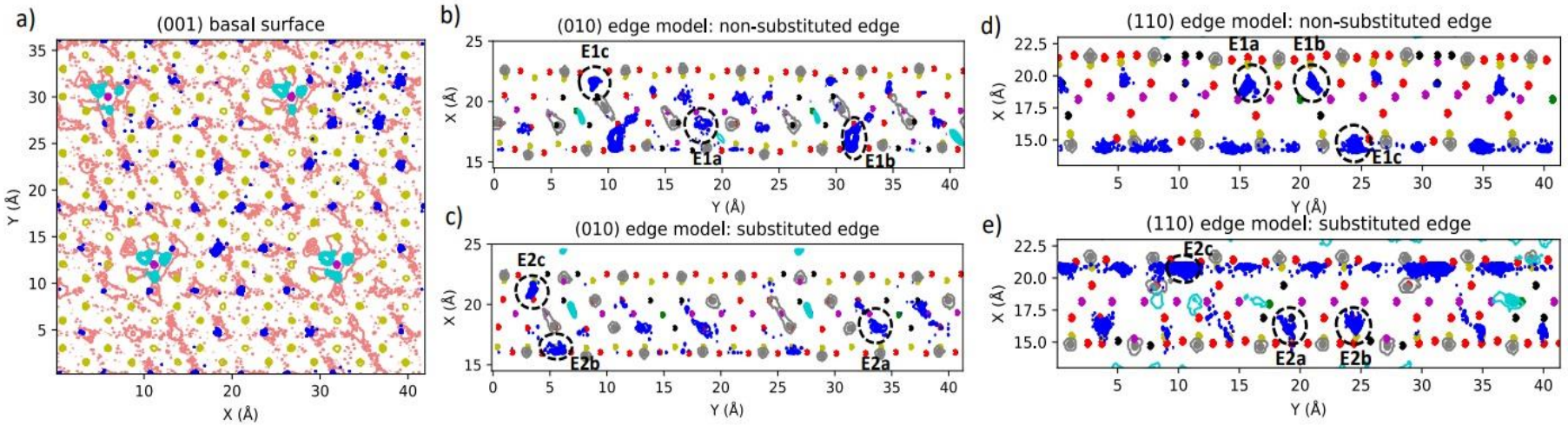
S.V.Kraevsky et al. 2020) *Applied Clay Science*, **186,** 105442.

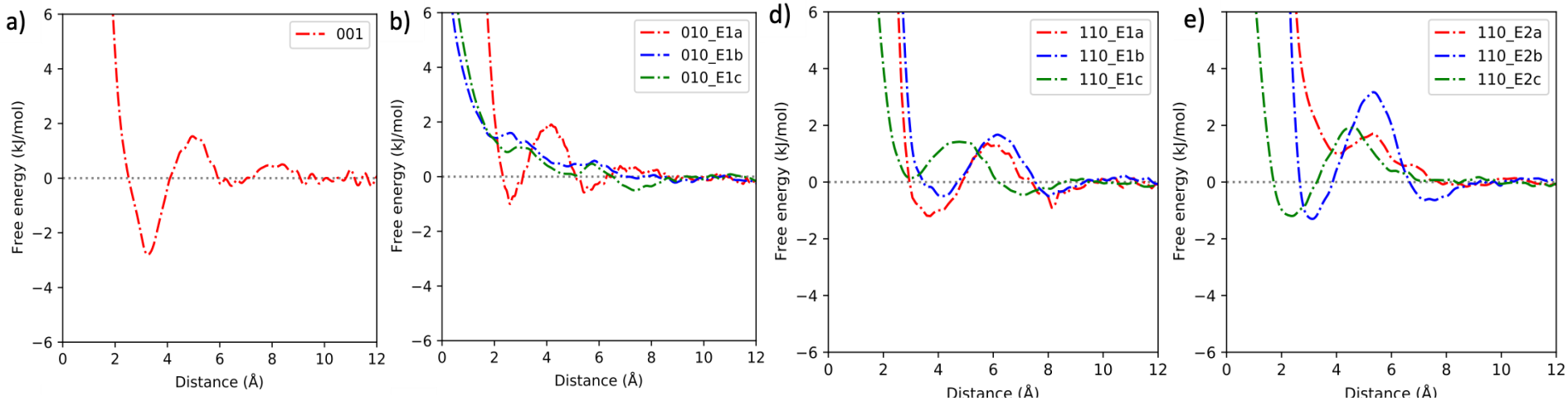
D.I.Grekov et al. (2020) *Phys.Chem.-Chem.Phys*, **22**, 16727-16733

N.Loganathan et al. (2020) *J.Phys.Chem. C,* **124**, 2490−2500

D.I.Grekov et al. (2021) *J.Phys.Chem. C,* **125**, 11499−11507

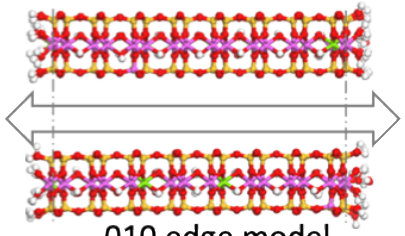
H_2 Gas Adsoption on Different Clay Surfaces



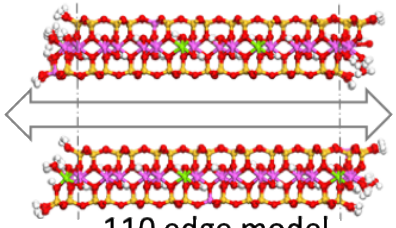


S. Mutisya, A.G. Kalinichev (2024) *J. Phys. Chem. C*, in preparation

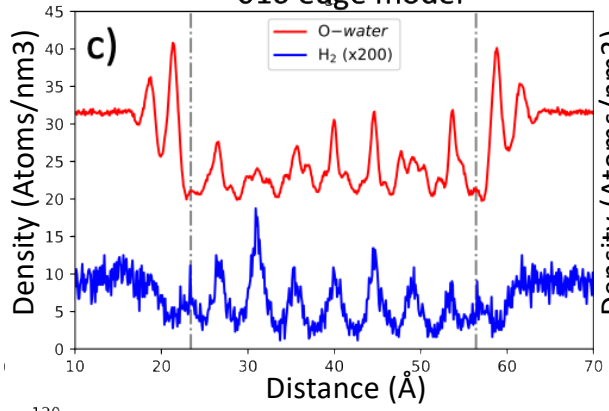
H_2 Gas Adsoption on Different Clay Surfaces

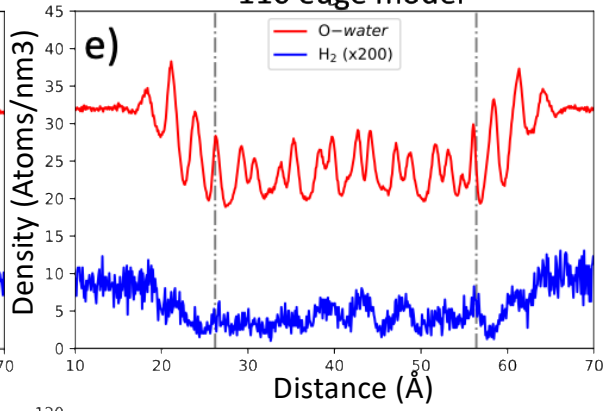


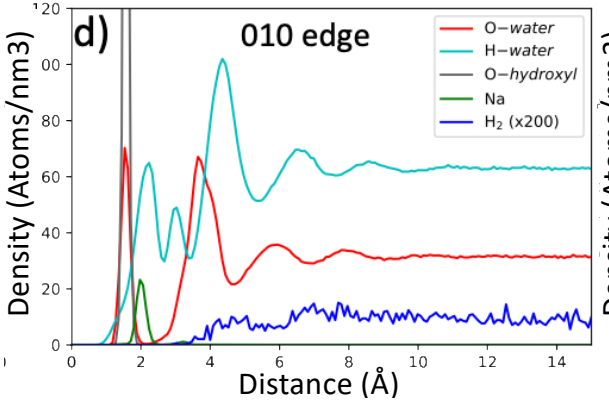
010 edge model

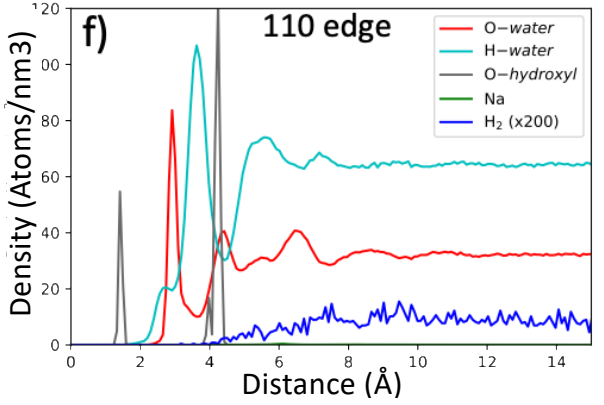


110 edge model

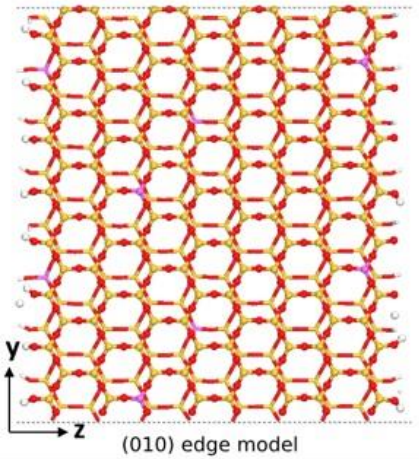




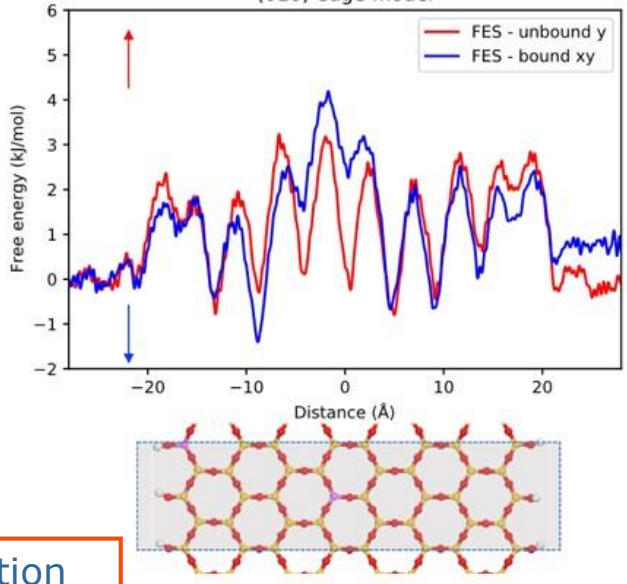




(010) Edge model



(010) edge model



S. Mutisya, A.G. Kalinichev (2024) *J. Phys. Chem. C*, in preparation

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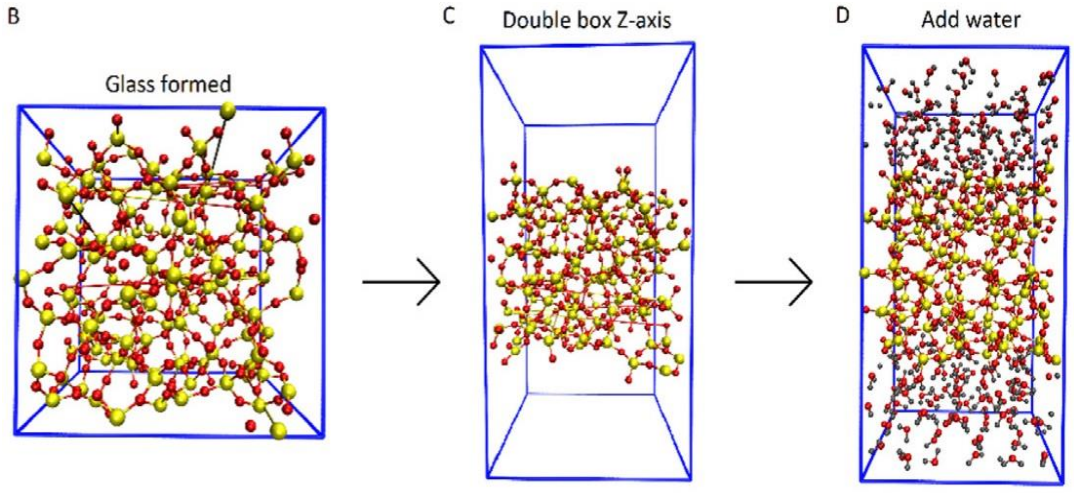
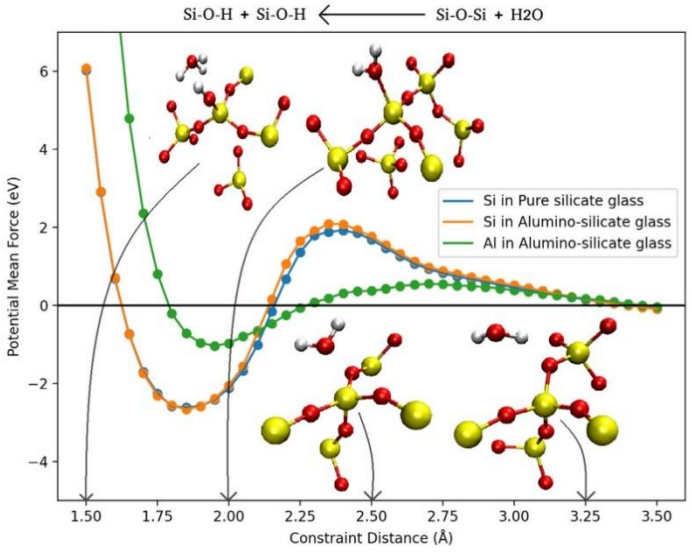
Molecular Modeling – External Collaborations (1)

CEA Marcoule – molecular mechanisms controlling the rate of alteration and chemical durability of nuclear waste glass.

PhD thesis co-advised by AGK:

Kamalesh DAMODARAN, 09/2020 - 12/2022;
Sumit TIWARI, 10/2022 - 10/2025

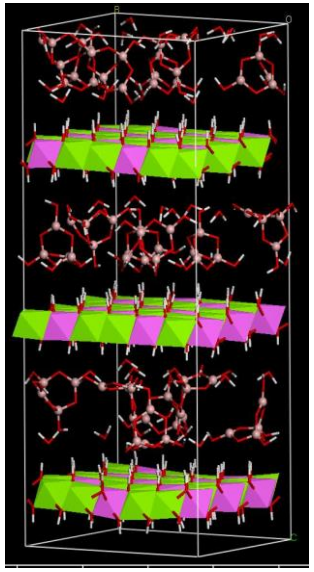




K. Damodaran, J.-M. Delaye, A.G. Kalinichev, S. Gin (2022) Deciphering the non-linear impact of Al on chemical durability of silicate glass. *Acta Materialia*, **225**, 117478.

Molecular Modeling – External Collaborations (2)

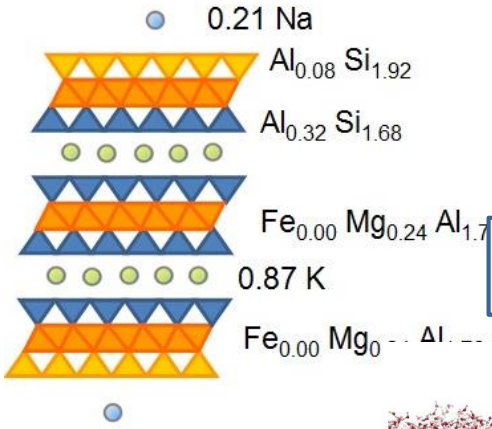
Turkey (*Department of Chemistry, Hacettepe University)* – layered double hydroxides (LDHs) - anionic clays for environmental and medical applications

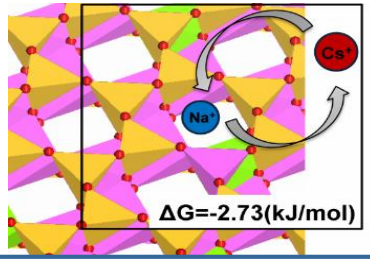


Synthesis, characterization, and MD simulations of Mg-Al-LDH intercalated with tetraborate anions for application for boron neutron capture therapy (BNCT) – potential brain cancer treatment using ^{10}B isotope delivered close to tumor cells

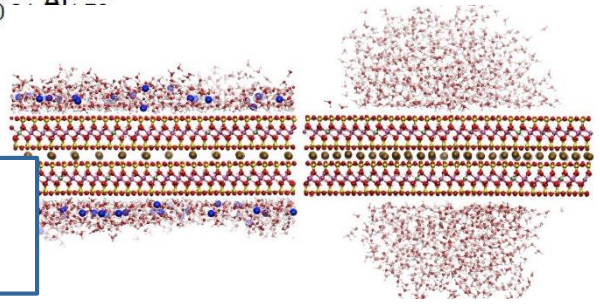
A.N.Ay, B.Zumreoglu-Karan, A.G.Kalinichev, V.Rives, R.Trujillano, A.Temel (2020) *Journal of Porous Materials*, **27**, 735–743

Poland (*Institute of Geological Sciences, Polish Academy of Sciences* – development of I/S COx models; hydrophobicity of smectites; clay-organic interactions





Cs^+/Na^+ exchange in interstratified I/S (COx)



Molecular nature of clay surface hydrophobicity

M.Szczerba, A.G.Kalinichev, M.Kowalik (2020) *Appl. Clay Sci.*, **188**, 105497

Z.Chen, N.Loganathan, M.Szczerba, G.Montavon, A.G.Kalinichev (2024) *Env. Sci. Technol*, in revision

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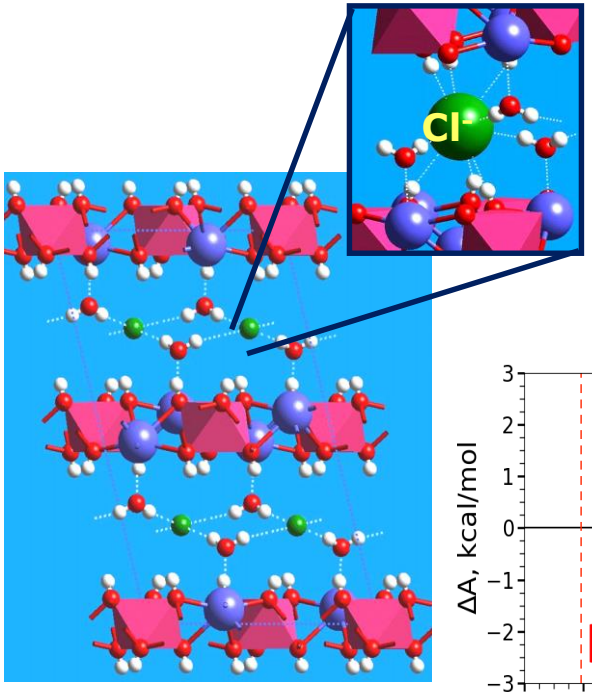
Molecular Modeling – External Collaborations (3)

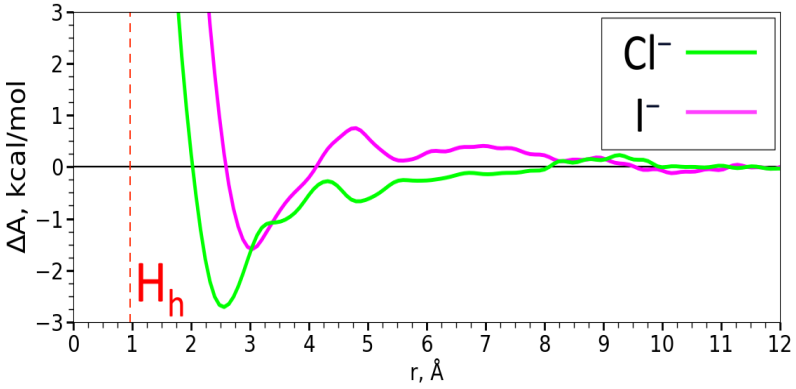
Russia (*International Laboratory for Supercomputer Atomistic Modelling and Multi-scale Analysis, National Research University Higher School of Economics, Moscow*) – atomistic simulations of clay-related and cement-related systems

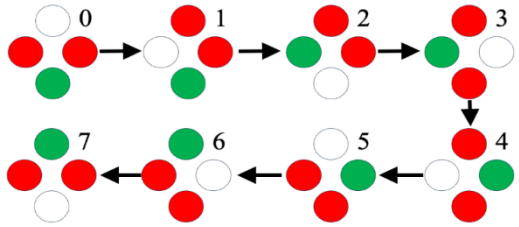
Calcium aluminates (*AFm cement phase*) as potential *adsorbents for anionic radionuclides* ($^{36}Cl^-$, $^{129}I^-$): $[Ca_2Al(OH)_6]\,X{\cdot}2H_2O$, X = Cl^-, I^-

Terminated in March 2022 due to the war in Ukraine



E.V.Tararushkin et al. (2022) *Cement and Concrete Res.*, **156**, 106759.
V.V.Pisarev et al. (2022) *Journal of Molecular Liquids*, **366**, 120290
M.A.Logunov et al. (2022) *Polymer Science A*, **64**, 908-917
E.V.Tararushkin et al. (2023) *Materials*, **16**, 5026.
E.V.Tararushkin et al. (2023) *Minerals*, **13**, 408.
E.V.Tararushkin et al. (2023) *Minerals*, **13**, 1018.
A.A.Glushak et al. (2024) *Appl. Geochem.*, under review.





● anion site ● H_2O site

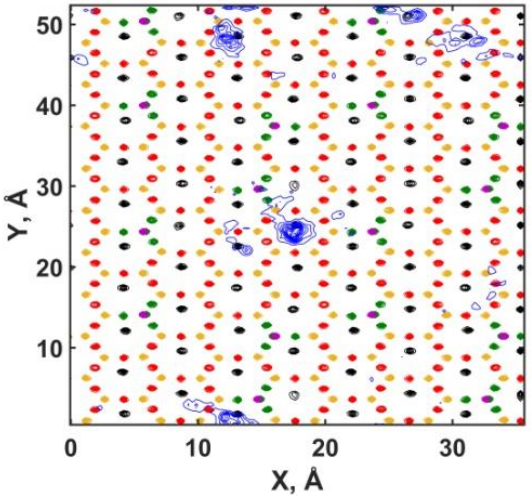
Molecular Modeling – External Collaborations (4)

Russia (*International Laboratory for Supercomputer Atomistic Modelling and Multi-scale Analysis, National Research University Higher School of Economics, Moscow*) – atomistic simulations of clay-related and cement-related systems

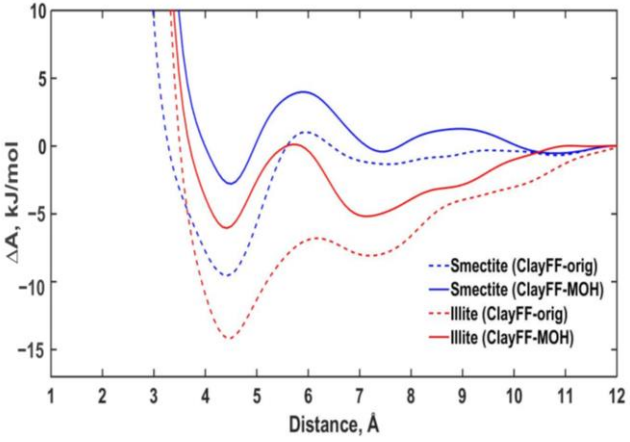
Uranyl adsorption at the hydrated clay surfaces

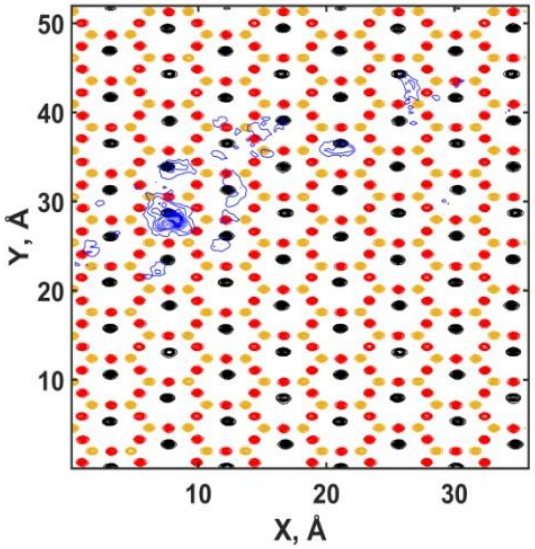
Terminated in March 2022 due to the war in Ukraine

Illite $K_{1.3}(Al_{3.5}Mg_{0.5})[Si_{7.2}Al_{0.8}]O_{20}(OH)_4$



Smectite $[Ca(H_2O)_6]_{0.4}(Al_{3.2}Mg_{0.8})[Si_8]O_{20}(OH)_4$





A.D.Krot, I.E.Vlasova, E.V.Tararushkin, A.G.Kalinichev (2024) *Minerals*, **14,** 109.

Molecular Modeling – Links to Experiment

Molecular-level understanding of metal ion retention in clay-rich materials

Xiandong Liu[1,2]✉, *Christophe Tournassat*[3,4]✉, *Sylvain Grangeon*[5], *Andrey G. Kalinichev*[6], *Yoshio Takahashi*[7] and *Maria Marques Fernandes*[8]

Author addresses

[1]State Key Laboratory for Mineral Deposits Research, School of Earth Sciences and Engineering, Nanjing University, Nanjing, China.
[2]Frontiers Science Center for Critical Earth Material Cycling, Nanjing University, Nanjing, China.
[3]Institut des Sciences de la Terre d'Orléans, Université d'Orléans–CNRS–BRGM, Orléans, France.
[4]Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, CA, USA.
[5]BRGM, Orléans, France.
[6]Laboratoire SUBATECH, Institut Mines-Télécom Atlantique, Nantes, France.
[7]Department of Earth and Planetary Science, The University of Tokyo, Tokyo, Japan.
[8]Laboratory for Waste Management, Paul Scherrer Institute, Villigen, Switzerland.

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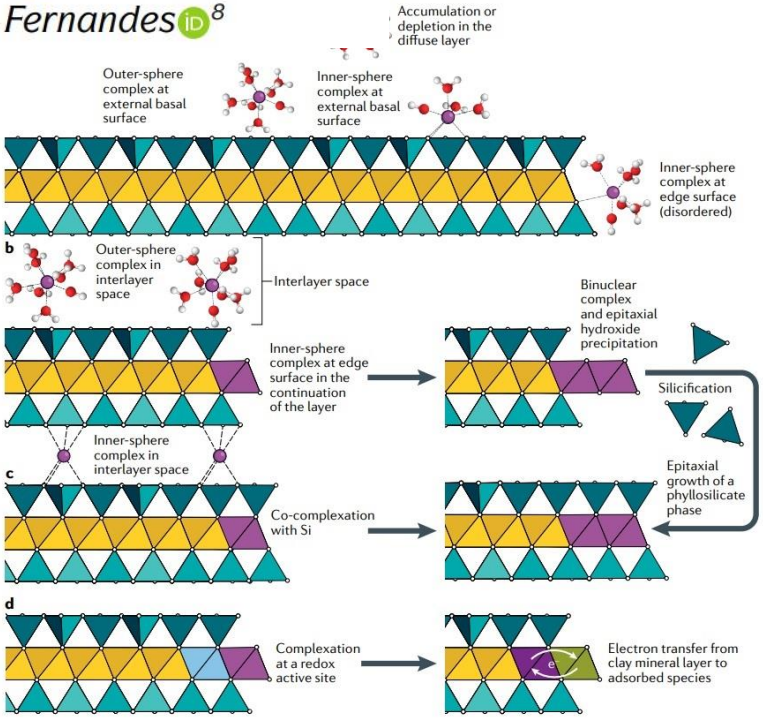
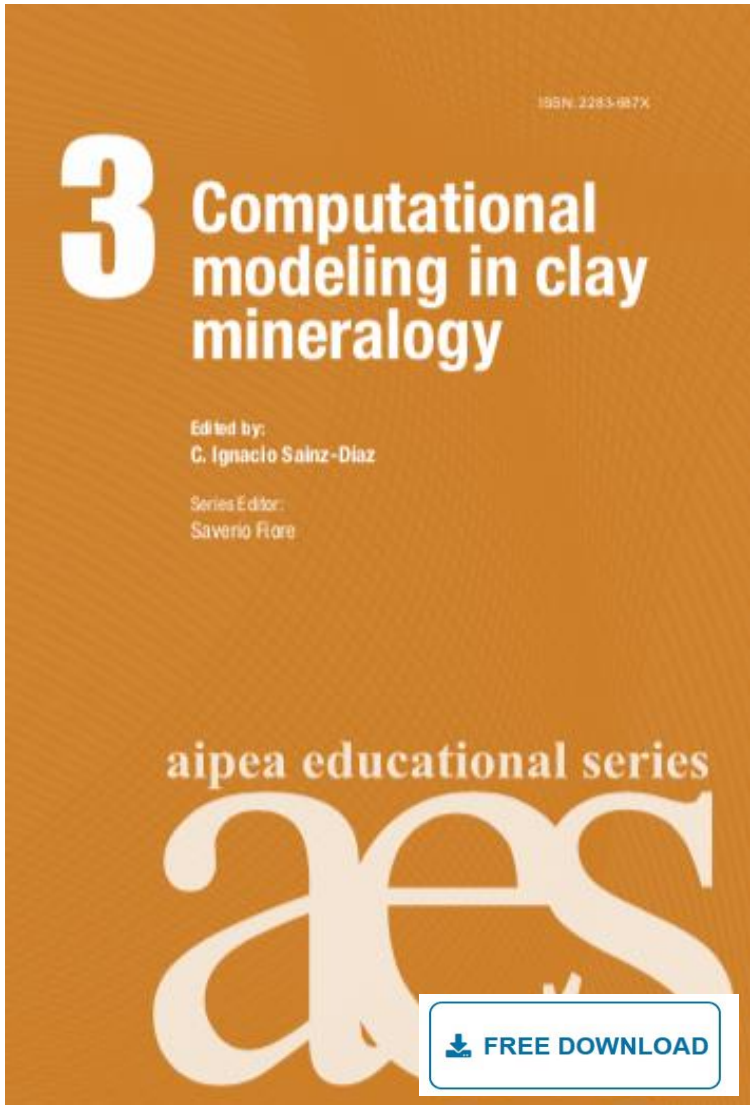


X.Liu et al. (2022) *Nature Reviews Earth & Environment* **3**, 461-476.

Molecular Modeling – Methods Development



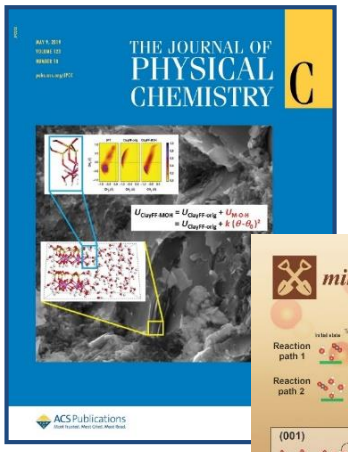
CONTENTS

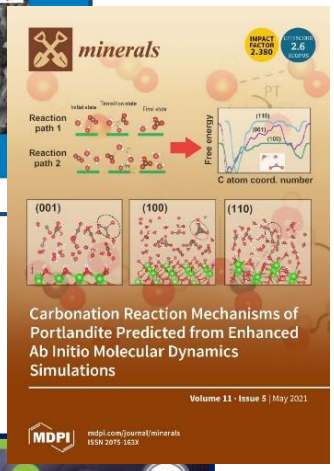
https://aipea.org/aes-books/

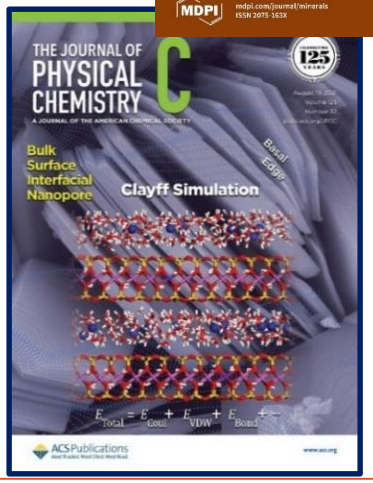
Molecular Modeling – Research Output

International dissemination activities (2019-2024)

- ✓ 25 publications in high quality peer-reviewed journals
- ✓ 3 publications were featured on the journals' covers
- ✓ 11 invited lectures and talks at major international conferences (Goldschmidt, ACS, CMS, ICC, Migration)
- ✓ 43 other oral and poster presentations at major international conferences
- ✓ 7 publications in preparation
- ✓ A.Kalinichev co-organized 4 special sessions/symposia at major international conferences
- ✓ In 2019-2020 A.Kalinichev was elected and served as the President of the Clay Minerals Society
- ✓ A.Kalinichev is also currently:
  - Editor-in-Chief of the section *Clays and Engineered Mineral Materials* of the journal *Minerals*
  - Assoc. Editor of the journal *Clays and Clay Minerals*
  - Assoc. Editor of the journal *Frontiers in Nuclear Engineering*
  - Assoc. Editor of the journal *Discover - Minerals*







Molecular Modeling – Perspectives for 2024-2029

- ✓ PhD project of ***Jakub Licko*** simulating the ***effects of small organic molecules on the adsorption and mobility of actinyls in clay*** will continue through 2024-2025.
- ✓ ***H_2 gas*** in different (un)saturated clay and cement systems for the problems of ***geological nuclear waste disposal***. This is thematically strongly linked with the new ***EURAD-GAS*** project and collaboration with colleagues at University of Grenoble. This work will be also extended to other technological applications, such as ***underground H_2 gas storage***.
- ✓ ***Collaboration with US colleagues*** (Sandia National Labs, Michigan State University) on the ***development of the ClayFF force field*** will continue by potentially including the effects of chemical reactivity at the clay and cement particle edges. With the arrival of ***Sébastien Le Crom*** – an expert in the polarizable force field development and application (***PIM***) – we may venture into adding the effects of polarizability to the current version of ClayFF.
- ✓ A new MD-simulation project to quantify the ***effects of soil organic matter on the mobility of Ra^{2+} in the environment*** is currently being developed in collaboration with ***Gilles Montavon*** at Subatech.
- ✓ The collaboration with ***CEA Marcoule on the atomistic simulation of nuclear waste glass*** corrosion and durability will continue at least through the end of 2025.
- ✓ New PhD project on ***molecular modeling of CO_2 mineralization*** is beginning in the fall of 2024 in collaboration with ***Sébastien Le Crom*** and ***Jean-François Boily*** (Umeå University, Sweden) in the framework of the SEED program at IMT Atlantique.
- ✓ A new collaborative project "***High fidelity multiscale solute transport modelling in nano-porous media under fluctuating thermodynamic and saturation conditions***" is currently being developed in collaboration with colleagues from the Geological Survey of Finland and the University of Helsinki.

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