



Contribution ID: 1007

Type: Oral Presentation

## Structure and adsorption mechanisms of hydrogen gas on water-saturated montmorillonite clay: A molecular dynamics study

Thursday, 25 May 2023 09:15 (15 minutes)

Radioactive waste arising from the production and use of radioactive materials calls for a sustainable waste management system which guarantees long-term safety to human and environment. To this end, a multi-barrier deep geological storage system consisting of both natural geological formations and engineered barriers has been proposed by several countries as a viable concept to store intermediate and high level wastes [1-3]. One of the central issues in the quantitative assessment of the integrity of a deep geological repository is gas generation and migration. Hydrogen ( $H_2$ ) gas, resulting from the anaerobic metal corrosion and water radiolysis processes is the most significant gas expected after the closure of the facility. Clay minerals, which are abundant in these geological sites, exhibit an intricate atomic structure with different polar species able to interact with  $H_2$  gas. In this study, we explore the structure and energetics of  $H_2$  gas adsorption on the interlayer, basal and edge surfaces of a montmorillonite clay model using molecular dynamics simulations. A special focus is given on the effects of local compositional and structural heterogeneity of montmorillonite. The simulation results show that on the basal surfaces,  $H_2$  occupies the siloxane cavities with the Al/Si isomorphic substitutions on the tetrahedral sheet limiting the occupation of those sites. A detailed analysis on the edge surfaces reveal that the local structure of water governs the adsorption energetics of  $H_2$  on the edges and within the interlayer pores.

### References

1. Andra, D. (2005). Synthesis: Evaluation of the feasibility of a geological repository in an argillaceous formation (2005).
2. Société coopérative nationale pour l'entreposage de déchets radioactifs (Suisse), & Johnson, L. (2002). Project Opalinus Clay: safety report: demonstration of disposal feasibility for spent fuel, vitrified high-level waste and long-lived intermediate-level waste (Entsorgungsnachweis). Nagra.
3. Neerdael, B., & Boyazis, J. P. (1997). The Belgium underground research facility: Status on the demonstration issues for radioactive waste disposal in clay. Nuclear Engineering and Design, 176(1-2), 89-96.

### Participation

In-Person

### References

### MDPI Energies Student Poster Award

No, do not submit my presentation for the student posters award.

### Country

France

## Acceptance of the Terms & Conditions

[Click here to agree](#)

## Energy Transition Focused Abstracts

**Primary author:** Dr MUTISYA, Sylvia M. (SUBATECH (IMT-Atlantique, Université de Nantes, CNRS-IN2P3) Nantes, France)

**Co-author:** Prof. KALINICHEV, Andrey G. (SUBATECH (IMT-Atlantique, Université de Nantes, CNRS-IN2P3) Nantes, France)

**Presenter:** Dr MUTISYA, Sylvia M. (SUBATECH (IMT-Atlantique, Université de Nantes, CNRS-IN2P3) Nantes, France)

**Session Classification:** MS13

**Track Classification:** (MS13) Fluids in Nanoporous Media