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Molecular Storytelling: Visualizing Geochemical Processes towards a Low-Carbon Society through Virtual Reality

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The transition to a sustainable low carbon society needs innovative approaches to address global challenges such as carbon capture and storage (CCS). This study explores the potential of molecular storytelling, coupling Molecular Dynamics (MD) simulations with Virtual Reality (VR), to visualize and communicate complex geochemical processes involved in CCS. We present immersive visualizations of three key systems: (i) CO2 up taken in clay minerals for carbon sequestration and long-term carbon storage [1]; (ii) CO2, CH4, and N2 gas diffusion within carbon nanotubes, demonstrating the potential for gas separation in natural and flue gases treatment [2]; and (iii) carbon dioxide diffusion in zinc-based metal-organic frameworks (MOFs), showcasing the versatility of MOFs in gas storage and separation and (iv) unraveling the rapid CO2 mineralization on basalts [3]. By transforming MD simulations into didactic VR experiences, we aim to enhance public and scientific understanding of these geochemical processes, fostering engagement and innovation in sustainable technologies. The videos that are produced, accessible without VR equipment, offer a scalable tool for education and outreach, bridging the gap between advanced computational modeling and real-world applications in geochemistry for a sustainable society.

[1] Miranda et al., Applied Surface Science 671, 160659 (2024)

[2] Miranda et al. Langmuir 39 (14), 4895-4903 (2023)

[3] Miranda et al. Scientific Reports 14 (1), 8116 (2024)



Figure 1 - carbon nanotubes with different radius.

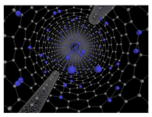


Figure 2 - inside a carbon nanotube with nitrogen gas

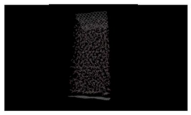


Figure 3 - boric acid in nanopores in a graphite sheet.

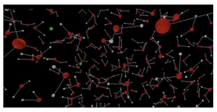


Figure 4 - lithium in a aqueous solution



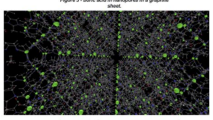


Figure 5 -porous metal-organic structures (MOF) formed by zinc ions with an organic ligand through which CO_2 is diffused.