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Computational and Topological Methods for In-situ Characterisation of Hetrogeneous Surface Wettability in Porous Media

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The efficiency of nano- and micro-porous materials in absorbing and releasing fluids, like CO_2 in geo-storage or water and gas in fuel cells and electrolyzers, depends on their surface wettability. Measuring wettability accurately is complex due to varying dynamic forces, chemical diversity, and surface texture. In situ measurements, which could assess wettability as a local contact angle (the angle at which a denser phase like water meets a solid in the presence of another phase like hydrogen, air, or CO_2), face challenges in precisely determining fluid curvatures, contact points, and the loops formed by multiphase fluids. We introduce a new, advanced topological method for in situ contact angle measurement and conduct a comparative analysis of existing geometric and topological techniques, evaluating their precision on ideal surfaces, CO_2-containing porous rocks, and water in gas diffusion layers. This novel approach offers more accurate and reliable in situ measurements for uniformly wetting environments compared to past topological methods, whereas geometric methods excel in mixed-wetting areas. Additionally, this research includes a detailed open-source platform for in situ wettability assessment in porous materials, which has significant implications for gas geo-storage, fuel cells, electrolyzers, filtration, and catalysis.

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References

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