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Microscopic Origin of Hysteresis in CH4 Sorption-Induced Deformed Coal Matrix: Insights from Stepwise Hybrid GCMC/MD Simulations

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CH4 sorption hysteresis is pivotal for predicting coalbed methane (CBM) production, yet its driving factor—the coupling of gas sorption and coal deformation—remains incompletely understood. Here, we use a stepwise hybrid grand canonical Monte Carlo/molecular dynamics (GCMC/MD) simulation technique to track continuous CH4 adsorption and desorption in a deformable coal matrix. Both matrix internal rearrangement and swelling contribute to pronounced sorption hysteresis and pore structure hysteresis. At the same chemical potential, pore size distribution and 3D pore space visualizations clearly show that the matrix fails to revert to its original configuration upon unloading, indicating structural irreversibility. Using free energy perturbation (FEP) method, we compare the free energy difference required to detach adsorbed gas (the energy barrier) and find that CH4 remains more strongly confined in local energy minima on the desorption path, even at lower loadings, leading to consistently higher free energy difference values (200~237 kBT) than on the adsorption path (165~225 kBT). These findings underscore how irreversible matrix rearrangements and deeper local minima along the desorption route drive persistent sorption hysteresis. Overall, our results highlight the necessity of incorporating sorption-induced deformation and structural hysteresis into predictive models of gas transport and storage in deformable coal.

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References

Primary authors: Mr YANG, Quanlin (University of Alberta); JIN, Zhehui (University of Alberta)

Presenter: JIN, Zhehui (University of Alberta)

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