Study of the effect of Surface Defects on Hydrophobicity at Rare-Earth Oxide–Water Interfaces using Molecular Dynamics simulation driven by ab initio-based high-dimensional neural network potentials

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Abstract: Water/solid interfaces have attracted significant attention due to central role in many fields, such as electrochemistry, corrosion, and heterogeneous catalysis. To enhance the performance of the materials under harsh environments, from reducing ice adhesion, to eliminating corrosion, hydrophobic materials have immense potential. General organic materials are hydrophobic, but they are easy to deteriorate and not durable. Recently, rare-earth oxides (REOs) are reported to be intrinsically hydrophobic due to saturation of electrons in the outer shell and lower tendency to form hydrogen bond. However, surface defects, like adatoms, and vacancies, are ubiquitous, which may change the hydrophobicity due to increasing surface reactivity and attracting structural arrangements. However, most of the experimental and computational studies about water/solid interfaces focus on ideal surfaces. Here, we propose to investigate the influence of the defects on hydrophobicity in knowledge with molecular dynamics simulation and identify candidate with durable hydrophobicity even with the presence of defects.