On the Chemistry at Oxide/Water Interfaces: the Role of Interfacial Water

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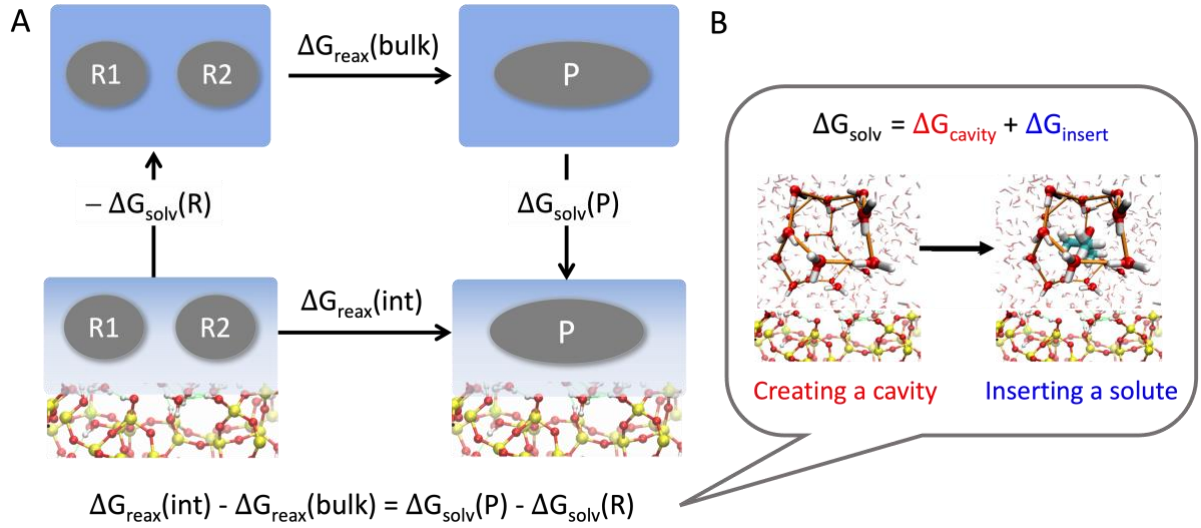
Oxide-water interfaces host many chemical reactions in nature and industry. There, reaction free energies markedly differ from bulk. While we can experimentally and theoretically measure these changes, we are often unable to address the fundamental question: what catalyses these reactions? Recent studies suggest that surface and electrostatics contributions are insufficient to answer. The interface modulates chemistry in subtle ways. Revealing them is essential to understanding interfacial reactions, hence improving industrial processes. Here, we introduce a thermodynamic approach combined with cavitation free energy analysis to disentangle the driving forces at play. We find water dictates chemistry via large variations of cavitation free energies across the interface. The resulting driving forces are both large enough to determine reaction output and highly tunable by adjusting interface composition, as showcased for silica-water interfaces. These findings shift the focus from common interpretations based on surface and electrostatics, and open exciting perspectives for regulating interfacial chemistry.



References
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