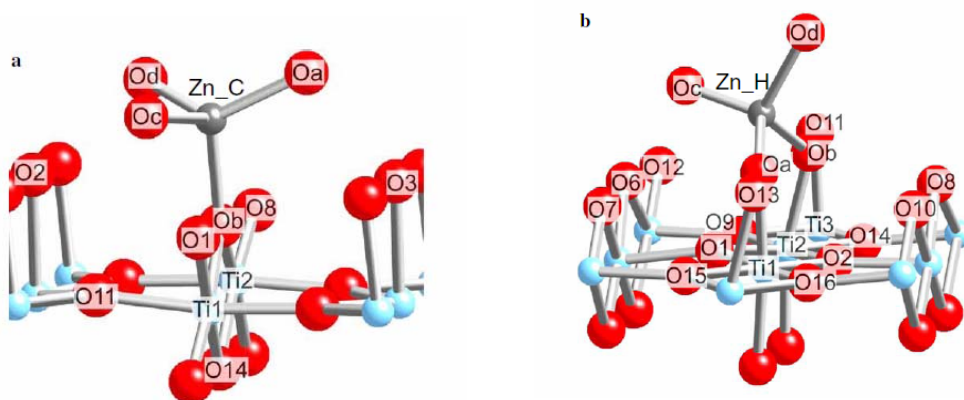


## Structure of $\text{Zn}^{2+}$ at the Rutile $\text{TiO}_2$ (110)-aqueous Interface

Z. Zhang, J. Catalano, P. Fenter, et al.



**Figure:** Adsorption geometry of adsorbed  $\text{Zn}^{2+}$  cations at the  $\text{TiO}_2$  rutile (110)-aqueous interface. Two distinct adsorption geometries are observed: monodentate above the bridging oxygen (left) and bidentate between terminal oxygens (right).

- Zhang et al. used a combination of X-ray standing waves, surface X-ray absorption spectroscopy and density functional theory to understand the adsorption of  $\text{Zn}^{2+}$  at the rutile ( $\alpha$ - $\text{TiO}_2$ ) (110)-aqueous interface. Previous studies had shown discrepancies between experimental and computational results suggesting that the interaction of the  $\text{Zn}^{2+}$  cation with the rutile-water interfaces was poorly understood.
- These results demonstrated that the hydration shell of the adsorbed  $\text{Zn}^{2+}$  cation is modified from that found in solution (from a 6-fold coordination environment in solution to a 4-fold coordination environment on the surface), and resulting in excellent agreement between all experimental and computational results.
- Density functional theory demonstrated that this transformation was directly coupled to the surface induced hydrolysis of the hydrated Zn cation.

**Reference:** Z. Zhang, P. Fenter, S.D. Kelly, J.G. Catalano, A. Bandura, J.D. Kubicki, J. Sofo, D.J. Wesolowski, M.L. Machesky, N.C. Sturchio, and M.J. Bedzyk, "Structure of Hydrated  $\text{Zn}^{2+}$  at the Rutile  $\text{TiO}_2$  (110)-Aqueous Solution Interface: Comparison of X-Ray Standing Wave, X-ray Absorption Spectroscopy and Density Functional Theory Results", *Geochimica et Cosmochimica Acta*, **70** 4039-4056 (2006).