

**Plenary Talk**

PLV VIII Thu 8:30 HSZ/AUDI

**Insights into aqueous solution oxide interfaces from ab initio neural network potential molecular dynamics** — ●ANNABELLA SELLONI — Princeton University, Department of Chemistry, Princeton, NJ, United States

Aqueous solution-oxide interfaces play a critical role in many environmental, biological, and energy-relevant processes. Molecular dynamics (MD) simulations employing ab initio based deep neural network po-

tentials (DPs) have recently emerged as a valuable approach to complement experimental observations and obtain detailed molecular scale insights. In this talk, I shall discuss recent applications of DP-MD to understand the structure and properties of aqueous solution-oxide interfaces. Focusing on titanium dioxide, a prototypical metal oxide with a prominent role in energy applications, specific topics will include characterization of the electrified TiO<sub>2</sub>-electrolyte interface, and the effects of organic compounds such as formic acid and methanol on the structure and chemistry of water at the interface.