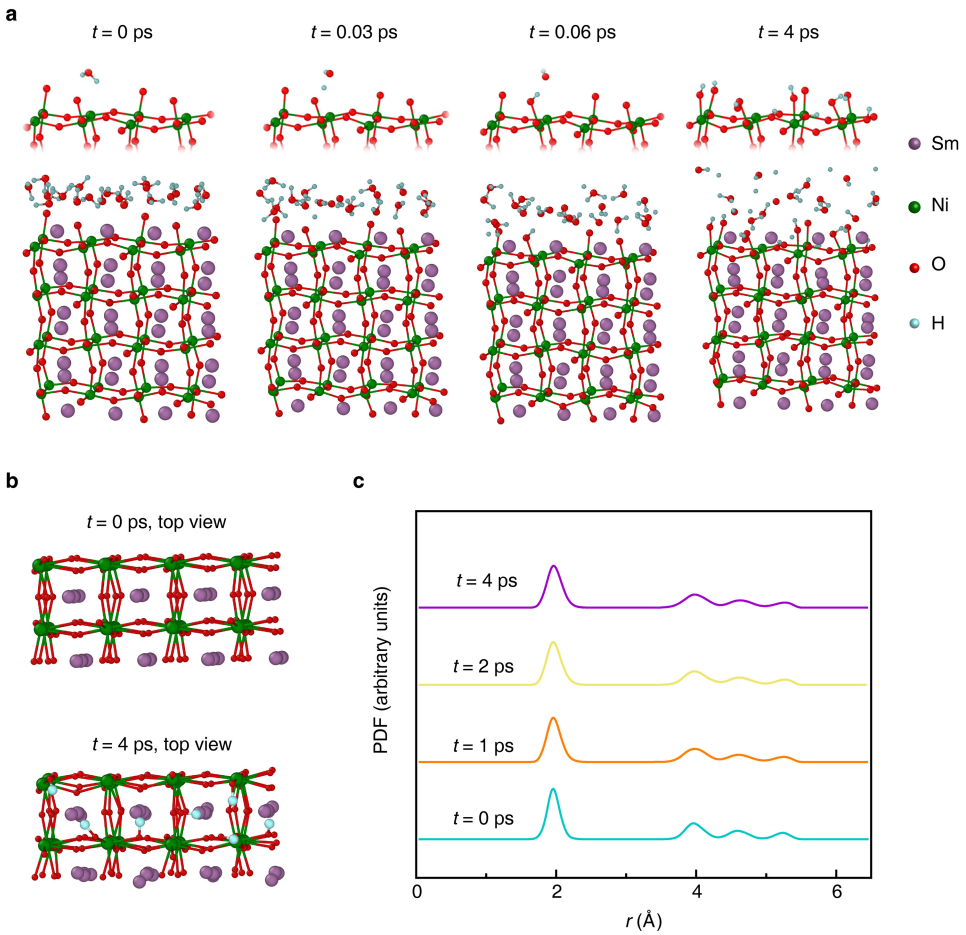

Extended Data Figure 9 | Dynamic simulations of SNO–water interactions at an elevated temperature of 500 K. a, Snapshots of the temporal evolution of a SNO surface submerged in water. Images tracking the evolution of a typical water molecule and the NiO_6 octahedra in the SNO layer closest to water are shown in the top panels. At 500 K, the surface protonation mechanisms are identical to those at ambient temperature, where water at the SNO surface dissociates into free protons and OH^-; a fraction of the free protons migrates to the oxide/water interface and binds to the surface oxygen of SNO. These atomic-scale processes observed in AIMD simulations support the proton accumulation and surface protonation mechanism depicted schematically in Fig. 1a. **b**, Top view, showing SNO protonation at the end of 4 ps. Compared with the pristine state at 0 ps, the SNO surface maintains structural stability during the protonation, even at 500 K (well above ocean temperature). **c**, The Ni–O pair distribution functions (PDF) calculated at various time intervals. The curves demonstrate well defined sharp peaks, suggesting that the SNO surface remains intact after surface protonation at elevated temperature in an aqueous environment. These results are consistent with the good stability inferred from the temperature-dependent electrical resistivity measurement of the submerged SNO samples.