Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Atomic coordinates for the optimized computational models and molecular dynamics trajectories. This file contains the plain-text atomic coordinates (x, y, z) of all optimized theoretical models used in the density functional theory (DFT) calculations (including bare Cu(100), BZA-Cu(100), and key reaction intermediates), as well as the initial and final structural configurations from the ab initio molecular dynamics (AIMD) simulations of the interfacial water network.