Supplementary Information

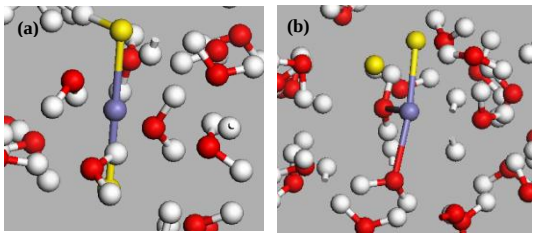

Figure 1: Car-Parrinello molecular dynamics (MD) simulations of FeS_2 in water: (a) configuration at t = 0 ps (b) final configuration at t = 2 ps.

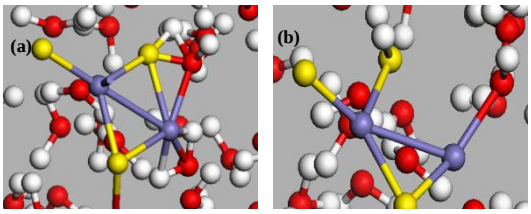

Figure 2: Car-Parrinello MD simulations of Fe_2S_3 in water: (a) intermediate configuration during simulation and (b) final configuration at t = 2 ps.

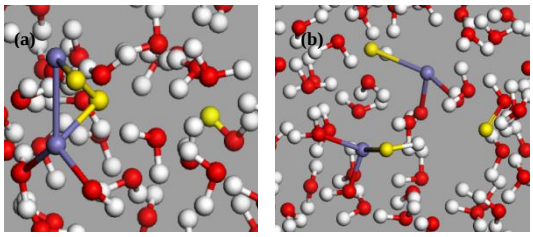

Figure 3: Car-Parrinello MD simulations of Fe_2S_2 in water: (a) intermediate configuration during simulation and (b) final configuration at t = 2 ps.

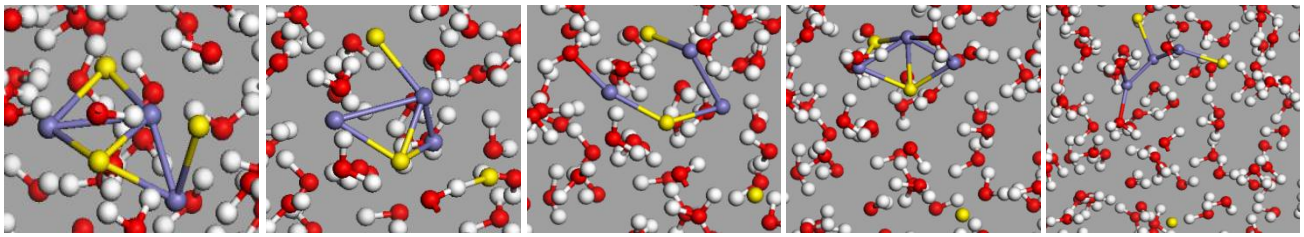

Figure 4: Snapshots taken during Car-Parrinello MD simulation of Fe_3S_3 in water.

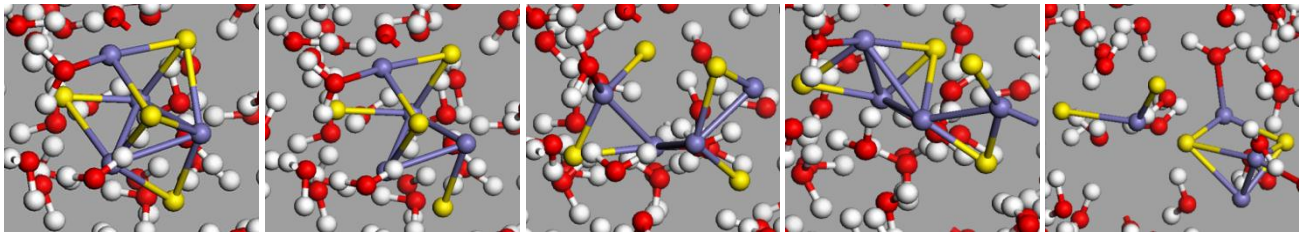

Figure 5: Snapshots taken during Car-Parrinello MD simulation of Fe_4S_4 in water.