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$_2$S$_3$ in water: (a) intermediate configuration during simulation and (b) final configuration at $t = 2$ ps.

Figure 3: Car-Parrinello MD simulations of Fe$_2$S$_2$ 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$_3$S$_3$ in water.

Figure 5: Snapshots taken during Car-Parrinello MD simulation of Fe$_4$S$_4$ in water.