Theory reveals the uncanny ways of cytochrome P450 to perform transformations like C-H hydroxylation, C=C epoxidation, heteroatom oxygenation, and C-C bond coupling, all via one active species! My talk will describe two-state reactivity (see Figure 1), proton coupled electron transfer (Figure 2), and catalysis by one or two water molecules, and cooperative reactivity.¹

Figure 1. Two-State Reactivity in P450 Hydroxylation.

Figure 2 Proton Coupled electron transfer.

References