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Theoretical investigations on the catalytic pathway of unspecific peroxygenases in the context of biocatalysis

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Biocatalysis has gained a reputation as sustainable alternative to conventional catalysis over the past years. Still, several limitations need to be addressed in order to make this method a competitive candidate for industrial applications. The catalytic activity of unspecific peroxygenases has been investigated in several experimental studies already, with promising results in terms of turn over rates and stability. Thus, our research focuses on the investigation of catalytic cycle of this enzyme class. As model proteins we have concentrated on *AaeUPO* and *CviUPO*, these heme-thiolate enzymes oxidize their substrate using H_2O_2 as co substrate. Using DFT calculations and QM/MM simulations of the whole enzyme system, we investigate how the molecular structure of the protein influences the energy barriers along the catalytic cycle. Furthermore, we want gain a deeper understanding of possible reaction channels for heme poisoning by additional hydrogen peroxide.

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