

# Catalytic degradation of nerve agents: QM and QM/MM Insight into water-regulation roles

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The nerve agents (NAs) are belong to highly toxic organophosphorus compounds, and their degradation has been receiving considerable attention. In hunting for efficient decontamination strategies toward NAs, the wild-type phosphotriesterase (PTE) enzyme, MOFs and MOF-functionalized materials, as well as metal oxides have been adopted, and they can hydrolyze or destruct these organophosphates. Here extensive QM & QM/MM calculations and MD simulations have been performed, and the plausible mechanisms for chemical and nonchemical steps, the roles of water molecules and key residues/groups in the enzymatic and heterogeneous catalysis have been discussed. The present results provide a comprehensive understanding of mechanistic details for the catalytic degradation of NAs by PTE, the postsynthetic modified M-MFU-4l-(OH) MOFs (M = Mn, Fe, Co, Ni, Cu, and Zn), CuO (111) and Cu<sub>2</sub>O(111) surfaces, which are important for development of high-performance catalysts towards the detoxification of nerve agents.

## References

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