

Atomistic Insights into Mercuric Ion Capture: Development of a Force Field and Application in Molecular Dynamics Simulations

Saskia Prusch^a, Philip Maier^a, Dirk Zahn^a

^a*Computer Chemistry Center, CCC, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nögelsbachstraße 25, 91052 Erlangen*

Removal from mercuric ions from aqueous environments is of considerable interest due to their severe environmental toxicity and their association with serious human health risks [1]. The strong affinity of mercuric ions to sulfhydryl groups has been widely exploited in medical treatment and engineered materials for efficient mercury capture[2]. However, molecular-level understanding of the underlying binding mechanism and structural dynamics remains limited. Molecular dynamics (MD) simulations provide an important tool for investigating such systems. Nevertheless, MD studies for transition metals systems are challenging because reliable force field parameters are often unavailable.

Here, density functional theory (DFT) calculations were employed to establish a foundation for developing a force field specifically tailored for the interaction between mercuric ions and sulfur. After parameter fitting and validation, the resulting force field was implemented in molecular dynamics simulations. The local environment of mercuric complexes were investigated using the ‘local pK’ concept to get insights into the overall charge [3].

Insights obtained from small complexes were subsequently transferred to larger systems. In particular, nanoparticles functionalized with self-assembled-monolayers (SAMs) containing sulfur groups were investigated to simulate the removal from mercuric ions from water.

REFERENCES

- [1] Yantasee, W, et. al., *Environmental science & technology*, **2007**, *41*, 5114–5119
- [2] Bjørklund, G., et. al, *Molecules*, **2019**, *24*.
- [3] P. Duchstein, et al., *CrystEngComm.*, **2025**, *10*, 1365-1512.