Towards rational design of organic copper corrosion inhibitors: High-throughput computational evaluation of adsorption energy

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Abstract Designing environment-friendly, high-efficiency, and low-toxicity copper (Cu) corrosion inhibitors is an important topic in the field of corrosion inhibitors. The current design of organic corrosion inhibitors mainly depends on empirical trial-and-error approaches. New methods are needed to accelerate and rationalize the design of corrosion inhibitors. The possible correlation between standard adsorption Gibbs energy and inhibition efficiency provides an opportunity for the rational design of corrosion inhibitors. A high-throughput computational framework is established for automatic computation of adsorption energies of organic corrosion inhibitors. A correlation between adsorption energies and changed Cu-d band centers induced by molecular adsorption is established. Standard adsorption Gibbs energies were derived based on additional thermodynamical and solvation correction. Standard adsorption Gibbs energy cannot be directly correlated with the inhibition efficiency. While some of corrosion inhibitors show linear correlation with standard adsorption Gibbs energies and inhibition efficiencies, the rest do not due to their orientation-dependent adsorption mechanisms.

Keywords Corrosion inhibitor，adsorption energy，density functional theory，high-throughput calculation