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Molecular dynamics studies of the adsorption behavior of methyl 3-((2-mercaptophenyl)imino)butanoate as corrosion inhibitors on copper surface

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ABSTRACT

High electrical conductivity and high surface quality of rolled copper foil (RCF) are often required simultaneously in flexible printed circuit boards (PCB). Surface oxidation and discoloration is a common quality defect in copper foil rolling production, significant improvement in corrosion protection can be achieved by addition of some specified corrosion inhibitors. Methyl 3-((2-mercaptophenyl)imino)butanoate (MMPB) as corrosion inhibitor for copper was studied by a combination of density functional theory (DFT) for the transferring electrons and molecular dynamics (MD) for the corrosion inhibitor and solvent. Results show that high efficiency of MMPB is mainly related with its azole, thiol functional groups, and carboxylate tail group form an adsorbed complex film over the surface of copper. The MD finds that the thiol group also improves the adsorptive interaction with the surface, as the carboxylate groups provide extra intermolecular attraction. The possibility of protonating MMPB to form neutral MMPBH is studied, and MD is used to assess their formation; we find that the translocation relies on the presence of inhibitors and also increases the electrical conductivity. The theoretical results show that the efficiency of the inhibitor accorded well with experimental results. A new design method is provided; it is possible to discover and design new inhibitor molecules in the metal processing industry and test the properties of a molecule using computer modelling.

KEYWORDS: rolled copper foil, corrosion inhibitor, density functional theory, molecular dynamics