# Calculated study on the influence of pollutants on the stability of corrosion products

**Wenjie Zhou**[1], Chaofang Dong[1], Dihao Chen[1], Yucheng Ji[1]

[1]*Beijing Advanced Innovation Center for Materials Genome Engineering, National Materials Corrosion and Protection Data Center, Institute for Advanced Materials and Technology, University of Science and Technology Beijing, Beijing, China.*

*zhouwenjie@xs.ustb.cn*

**Abstract** This study explores the influence of corrosion product layers on the protective properties of metal materials, particularly the effects of S and Cl ions on the structural stability of α - FeOOH and γ - FeOOH corrosion products. The influence of different anions on hydrogen bonding and charge density was studied by replacing the O atom in the crystal structure, and the corresponding infrared spectra were calculated. The results showed that although the substitution of S ions reduced the number of hydrogen bonds, the overall stability remained good, and some S-H bonds were enhanced; The substitution of Cl ions significantly reduces the number and strength of hydrogen bonds, while also disrupting the symmetry of the structure, resulting in a significant decrease in structural stability. We found that the effect of Cl ions on γ - FeOOH is much greater than that on α - FeOOH, while the effect of S ions on the two corrosion products is not significantly different.

**Keywords** corrosion product ; first principle calculation

## Reference

[1] Tian Lu, J. Chem. Phys., 161, 082503 (2024)