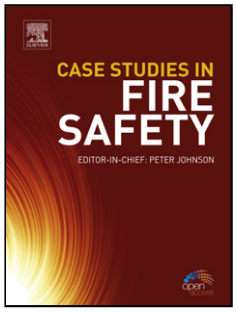

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PII: S0010-938X(17)31203-9
DOI: https://doi.org/10.1016/j.corsci.2018.03.009
Reference: CS 7425

To appear in:

Received date: 6-7-2017
Revised date: 1-2-2018
Accepted date: 7-3-2018

Please cite this article as: Wang H, Hao Y, Chen S, Cheng M, Li C, Sun S, Hu S, DFT study of imidazoles adsorption on the grain boundary of Cu (100) surface, *Corrosion Science* (2010), https://doi.org/10.1016/j.corsci.2018.03.009

DFT study of imidazoles adsorption on the grain boundary of Cu (100) surface

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Highlights

- The adsorption of three corrosion inhibitors on both Cu (100) grain boundary (GB) and ideal surface was studied by using density functional theory (DFT).
- The energy and active site of Cu (100) grain boundary surface were analysed.
- The atom charge, charge density difference and partial density of states were analysed.
- Two possible inhibition mechanisms of intergranular corrosion was summarized.

Abstract

Density functional theory was used to investigate the adsorption of imidazole (IMD), benzotriazole (BTAH) and 2-mercaptobenzoxazole (MBO) on the grain boundary (GB) of Cu (100) surface. Results show that molecules prefer to adsorb on the grain boundary with the larger distortion degree and more adsorption sites. The main interaction of molecules and grain boundary is chemisorption through C, N, S-Cu bonds in both perpendicular and parallel modes. Hydrogen bonds and the lateral dipole-dipole interactions are also found. Based on the adsorption behaviour, the coverage effect and charge redistribution might be two possible inhibition mechanisms of inhibitor molecules.