Adsorption of Benzene-1,4-diol, 3-Methyl-1,2-cyclopentanedione and 2,6-Dimethoxyphenol on aluminium (1 1 1) plane using density functional theory calculations (Article)

Mohamad Sidik, M.S., Abu Bakar, M.H., Allal, H.

Abstract:
The corrosion inhibitive actions of a few potential organic molecules extracted from rice husk bio-oil, namely benzene-1,4-diol, 3-methyl-1,2-cyclopentanedione, and 2,6-dimethoxyphenol, were investigated using first-principle calculation. Adsorption of these molecules on the aluminium (1 1 1) plane was simulated to unravel the inhibitor-surface bonding mechanism using a density functional theory with different adsorption sites and molecule geometry orientations. The electronic properties of the adsorption system also revealed the bonding mechanism and the different bonding characters between the three molecules. Based on the calculated adsorption parameters and electronic properties between inhibitor and surface atom, the 3-methyl-1,2-cyclopentanedione was discovered to be chemisorbed in both perpendicular and parallel geometry. It is pointed out that the π-system and oxygen lone pairs of 3-methyl-1,2-cyclopentanedione are rather important. Meanwhile, the benzene-1,4-diol and 2,6-dimethoxyphenol molecules were physisorbed in both geometries, and the bond lengths between oxygen and aluminium atoms are longer than the covalent radii of oxygen-aluminium. Finally, 3-Methyl-1,2-cyclopentanedione was identified as the most effective corrosion inhibitor to substantially reduce corrosion due to strong interaction with the aluminium surface.

ISSN: 3010104

DOI: 10.1016/j.chemphys.2022.111592

PUBLISHER: SCOPUS