عنوان مقاله:

Corrosion Inhibition of Iron Using Silicate Base Molecules: A Computational Study

محل انتشار:

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نویسندگان:

Usman Shehu - *Department of Pure and Industrial Chemistry, Faculty of Physical Sciences, Bayero University, Kano, Nigeria*

Bishir Usman - *Department of Pure and Industrial Chemistry, Faculty of Physical Sciences, Bayero University, Kano, Nigeria*

خلاصه مقاله:

The compounds in this research work were studied theoretically using computational methods to analyze the inhibition of the following compounds of silicate-based obtained from Tapinanthus Globiferus. Arsenous acid, tris(trimethylsilyl)ester, Cyclotrisiloxane, hexamethyl- and Silicic acid, diethyl bis(trimethylsilyl)ester on Fe surface as Parameters were studied using quantum chemical method through DFT and molecular dynamic simulations. Mild steel Fe (۱۱۱) was used due to its respective close-packed and dense atoms on the surface. The Fukui function and the local and global reactivity were calculated to give the molecule's reactivity. Based on the values of calculated adsorption .and binding energies. The mechanism of the molecules was inferred to exhibit Physisorption on the Fe surface

کلمات کلیدی:

Corrosion-inhibition, DFT, Silicate Based Compounds, Fe surface