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A combined experimental and electronic-structure quantum mechanics approach for studying the kinetics and adsorption characteristics of zinc nitrate hexahydrate corrosion inhibitor on the graphene oxide nanosheets

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Abstract: The adsorption mechanisms and kinetics of zinc cations at the graphene oxide (GO) nanosheets-water interface were studied by experimental and theoretical approaches. Results showed that adsorption of zinc cations onto GO surface forms a monolayer and obeys Langmuir isotherm. Meanwhile, the kinetics of sorption best fits with pseudo second order model, suggesting that the sorption process is more than one-step. Various characterization techniques such as Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), X-ray diffraction (XRD), ultraviolet-visible spectrophotometry (UV-Vis) and field emission scanning electron microscopy (FE-SEM) equipped with energy dispersive X-ray spectroscopy (EDS) were conducted to describe the mechanism of adsorption process. EIS and polarization

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