

Abstract Submitted  
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**Study on the Corrosion Protection of Paint Coating with Eco-Friendly Inhibitors** MEGAN CUI, RICHARD KYUNG, CRG-NJ — Computational modeling and simulations are efficient methods for understanding corrosion and corrosion protection. Based on the physical, chemical and thermodynamic properties of materials, making predictions of corrosion was presented in this paper. To inhibit material corrosion such as metallic or paint corrosion, this paper have focused on finding either naturally-made or artificially modified compounds that can prevent these oxidation and corrosion. Due to its anti-corrosion performance, phytoncide molecules have been found to impact the growth of rustic or oxidized molecules. Since the anticorrosion and antimicrobial potency and range of phytoncides vary greatly among agents, activity of various antioxidant components of extracts were studied. The reactivity and conductivity have been measured through the dipole moments to calculate the activity level the molecule could have with other nearby molecules. Also, electrostatic potential maps were utilized to visualize the polarization and assess the reactivity level of each molecule. The benefit of modeling corrosion using the computational simulations is that the design and optimization can be done quickly and at a lower cost, which also lowers the risk of expensive redesigns occurred in the laboratory experiment.

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