

## An experimental and theoretical study black cumin seed extract as environmentally sustainable corrosion inhibitors

Experimental corrosion tests and theoretical calculation were conducted to investigate the corrosion inhibition mechanism of black cumin seed (BCS) extract for copper in 1 M H<sub>2</sub>SO<sub>4</sub> solution. Electrochemical testing using electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) method showed that BCS adsorbed to form a protective layer on the copper surface with high inhibition efficiency at 500 ppm concentration (73,35%). The BCS is a mixed inhibitor (anodic and cathodic) that adsorbs physically on the copper surface and obeys the Langmuir isothermal adsorption model. Quantum chemical calculation and molecular dynamic simulation show that the studied BCS molecules adsorb strongly on the copper surface with parallel orientation mode. The methyl linoleate molecules from BCS produce the most stable adsorption energy of the other studied compound molecules as a result of molecular dynamic simulation.

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