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Molecular modeling in the use of amino acids as corrosion inhibitors on nickel surfaces

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Among a list of important metals, nickel occupies a prominent place for being present in the composition of various metallic alloys, such as stainless steel itself. It gets all this credit for being primarily responsible for the stable austenitic structure and contributing substantially to the alloy's corrosion, oxidation resistance, and mechanical properties throughout the usable temperature range. This corrosion resistance of nickel occurs due to the formation of a passive oxide layer on its surface when exposed to corrosive media. However, nickel is not exempt and can be attacked by acidic media at a considerable rate in the industry. Thus, its corrosion rate must be controlled to avoid accidents or production losses. One of the widely used corrosion control methods is the addition of corrosion inhibitors. Nonetheless, the big problem is that most available inhibitors are toxic compounds. There is a tendency to replace these toxic inhibitors with new ecologically correct inhibitors, and amino acids have occupied a prominent place in this change in the last two decades. They are non-toxic, biodegradable, relatively inexpensive, and completely soluble in aqueous media. In recent years, a growing range of corrosion scientists has used quantum chemical calculations to understand the interaction of anticorrosives on metal surfaces. Some amino acids have been tested as corrosion inhibitors using semi-empirical methods and DFT (Density Functional Theory), but no DFT study of all amino acids as nickel corrosion inhibitors has been reported in the literature. Therefore, in this study, we propose the evaluation of the adsorption of twenty amino acids on a pure nickel surface through molecular modeling calculations. For this, we built and optimized a unit cell with six layers of nickel using the CASTEP software. Then we performed a conformational search at the classical level of each amino acid on the surface of the nickel using the Universal force field implemented in the FORCITE software to determine the configuration's lowest energy so that we could rank the amino acids by their interaction energies. In addition, we obtained the quantum chemical descriptors, such as the energy of the highest occupied molecular orbital HOMO, the energy of the lowest unoccupied molecular orbital LUMO using GGA/B3LYP through the Dmol3 software, and the energy intervals Delta E were calculated.