Chapter 2
A Computational Protocol for the Study and Design of Effective Organic Corrosion Inhibitors: An Overview

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ABSTRACT

While traditional corrosion scientists design new corrosion inhibitors through structural modification and testing hundreds of compounds in the lab with practical means that are costly in terms of time and materials, successive and continuous developments in hardware and software make the design process faster and cheaper. This chapter introduces a computational protocol to differentiate the performance of organic corrosion inhibitors. On the other hand, it can be used to design new anticorrosive inhibitors. Another aim of this chapter is to correct common mistakes in conducting computational calculations. The protocol includes three successive phases of calculations: I- DFT-examination of the reactivity of the isolated molecules before the adsorption process. II- Studying the physical adsorption of molecules on the metallic surface using Monte Carlo (MC) or molecular dynamics (MD) simulations. III- Studying the chemical adsorption of molecules on the metallic surface using density functional-based tight binding (DFTB) or periodic density functional theory (DFT) methods.

INTRODUCTION

The main reason for the corrosion of metals is their unbridled desire for the most stable state in terms of thermodynamics; therefore, they resort to interaction with the surrounding environment to achieve this. This urgent desire exposes our world to life and economic risks because metals are the basis for establishing facilities, equipment, and devices; therefore, vast losses happen. Therefore, scientists have

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worked for decades to combat this by finding various solutions to discourage the corrosion process. Two major approaches to protect metals or alloys from corrosion are well-established;

1. Isolating the surface from aggressive media using coatings or film-forming chemicals or
2. Offsetting the loss of electrons from corroded structure using cathodic protection by impressed current or by using active sacrificial anodes. Chemists have had an essential role in developing organic chemicals used as inhibitors.

Computers were used to study and understand physical and chemical phenomena in the 1950s (Jasim, 2020). Since then, computational chemistry and its applications have emerged in many areas, such as catalysis and corrosion. Although hardware limitations prevented researchers from simulating real systems until the beginning of 2000the s, this problem has been solved thanks to the development of computing power units (CPUs) and graphic processing units (GPUs). Due to the increasing use of molecular modeling and simulations, this chapter introduces a comprehensive computational protocol to give a complete picture bout the events at the surface.

Like wet laboratory experiments, molecular simulations and modeling are also computer experiments in which one controls the setting of calculations using commercial programs and preparing scripts and input files. The end goal of such a simulation is obtaining the equilibrium properties of the tested system. Molecular simulations and modeling, in principle, provide atomic details of the structures and motions. The Monte Carlo method and molecular dynamics are the most common molecular simulation methodology, while DFTB and the traditional periodic DFT are used for quantum chemical modeling.

This chapter introduces a complete computational protocol for investigating and/or designing new organic corrosion inhibitors. Although few papers (El-Hendawy et al., 2022) used it for this purpose, we emphasize that such protocol should be predominated to give a complete insight into the anticorrosive events at the metal surface and thermodynamics and kinetic properties. Scheme 1 summarizes the protocol procedure, which includes two main steps: working on the isolated molecule and working on the molecule/surface complex. The latter is used for studying physical and chemical adsorption.