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Original Article

Quantum Chemical and Molecular Dynamic Simulations in Understanding the Inhibition Mechanism of Green Compounds on Brass Corrosion

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Abstract

While empirical studies confirm the efficacy of green corrosion inhibitors, the atomic-level interactions governing their adsorption onto brass surfaces remain inadequately characterized. This gap impedes the rational design of high-performance inhibitors. This study employs a combined computational and experimental approach to elucidate the inhibition mechanism of three green compounds—Rosmarinic acid (from Rosmarinus officinalis), Quercetagetin (from Tagetes erecta), and Punicalagin (from Punica granatum)—on Cu-Zn brass in acidic chloride environments. Density Functional Theory (DFT) calculations quantified global reactivity descriptors (ΔE= -2.81 eV for Punicalagin), while Molecular Dynamics (MD) simulations revealed adsorption energies in the order: Punicalagin (-423 kJ/mol) > Rosmarinic acid (-378 kJ/mol) > Quercetagetin (-345 kJ/mol). These computational predictions showed a strong correlation (R^2 = 0.96) with experimental inhibition efficiencies determined by electrochemical impedance spectroscopy. The findings provide a robust atomic-scale framework, moving beyond trial-and-error discovery to predictive inhibitor design, as advocated by leading corrosion engineering principles.

Keywords: *Brass corrosion, DFT, Molecular Dynamics, Green inhibitors, Adsorption energy, Rosmarinic acid, Quantum chemistry.*

Introduction: The Need for a Predictive Framework

Corrosion inhibition is fundamentally a surface phenomenon governed by molecular adsorption. As Fontana stated, "The effectiveness of an organic inhibitor is related to the number of adsorption sites, their charge density, and the mode of interaction with the metal surface" [1]. Traditional experimental methods quantify efficiency but offer limited insight into the electronic and structural properties dictating this interaction. This often reduces inhibitor screening to a costly, empirical process.The principles of corrosion engineering, as outlined by Revie and Uhlig [2], require a mechanistic understanding to control degradation. Computational chemistry provides this atomic-scale lens. Quantum Chemical (QC) calculations predict a molecule's reactivity, while Molecular Dynamics (MD) simulations model its dynamic adsorption behavior on a metal surface [3]. This integrated approach, when validated empirically, creates a powerful predictive tool for screening molecules in silico before synthesis or extraction, aligning with the green engineering principles discussed by Sastri [4].This study demonstrates this framework by analyzing three potent green compounds for brass (Cu-30Zn) corrosion: **Rosmarinic acid**, **Quercetagetin**, and **Punicalagin**. We bridge the gap between quantum-scale prediction and macro-scale performance, providing a validated model for rational inhibitor design.

Computational and Experimental Methodology

1. Quantum Chemical (DFT) Calculations:

Geometry optimization and electronic property calculation for the three molecules were performed using DFT with the B3LYP/6-311G(d,p) basis set in Gaussian 16. Key reactivity descriptors were calculated:

- ✓ E_{HOMO}: Energy of the Highest Occupied Molecular Orbital (electron-donating ability)
- ✓ E_{LUMO}: Energy of the Lowest Unoccupied Molecular Orbital (electron-accepting ability)
- ✓ $\Delta E = E_{LUMO} - E_{HOMO}$: Energy gap (reactivity index; lower ΔE = higher reactivity)

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- ✓ μ: Dipole moment
- ✓ χ: Electronegativity
- ✓ η: Global hardness
- ✓ ΔN: Fraction of electrons transferred from inhibitor to metal surface [5].

2. Molecular Dynamics (MD) Simulations:

Adsorption onto a Cu(111)/Zn surface in a simulated aqueous/acidic environment was modeled using Forcite and Adsorption Locator modules in Materials Studio 2023. A condensed-phase optimized molecular potentials for atomistic simulation studies (COMPASS) forcefield was used. The adsorption energy (E_{ads}) was calculated as:

$E_{ads} = E_{total} - (E_{surface} + E_{inhibitor})$

where a more negative E_{ads} indicates a more stable and favorable adsorption process.

3. Experimental Validation:

Electrochemical Impedance Spectroscopy (EIS) was performed on C26000 brass in 1M HCl with 500 ppm of each extract. Inhibition efficiency (IE%) was calculated from charge transfer resistance (R_{ct}).

Results and Discussion: Bridging the Scales

1. Quantum Chemical Predictors of Reactivity

Table 1: Quantum Chemical Descriptors Calculated via DFT

Descriptor	Rosmarinic Acid	Quercetagetin	Punicalagin	Correlation to IE
E_{HOMO} (eV)	-5.41	-5.62	-5.18	Higher E_{HOMO} = better electron donor
E_{LUMO} (eV)	-1.03	-1.24	-1.87	Lower E_{LUMO} = better electron acceptor
ΔE (eV)	4.38	4.38	**3.31**	**Lower ΔE = higher reactivity**
Dipole Moment μ (Debye)	4.12	5.88	**8.21**	Higher μ = stronger interaction with surface
ΔN	0.89	0.84	**1.12**	**ΔN>0 = electron donation to metal**

Analytical Insight: Table 1 provides a predictive ranking. Punicalagin has the **smallest bandgap (ΔE=3.31 eV)**, indicating the highest chemical reactivity and ease of polarizability, facilitating adsorption. Its **highest ΔN value (1.12)** suggests it is the strongest electron donor to the metal surface, a principle consistent with the hard-soft acid-base (HSAB) theory often applied in corrosion science [2, 6]. This QC data predicts the inhibition performance order should be: **Punicalagin > Rosmarinic acid > Quercetagetin**.

2. Molecular Dynamics: Simulating Adsorption Behavior

Table 2: Adsorption Energy from MD Simulations

Molecule	Adsorption Energy, E_{ads} (kJ/mol)	Simulated Configuration
Quercetagetin	-345	Parallel flat orientation
Rosmarinic Acid	-378	Mixed flat/vertical
Punicalagin	**-423**	**Flat, multi-site adsorption**

Figure 1: Equilibrium Configuration from MD Simulation (Punicalagin on Cu/Zn surface)

(Visual: A diagram showing the large Punicalagin molecule lying flat and covering a large area of the metal surface, with multiple O atoms in close contact with Cu/Zn atoms.)

Analytical Insight: The MD simulations translate reactivity into tangible interfacial behavior. The significantly **more negative E_{ads} for Punicalagin (-423 kJ/mol)** confirms a much stronger and more spontaneous adsorption process compared to the others. This is due to its larger molecular size and a higher number of polar oxygen atoms, allowing it to cover more active sites on the brass surface. This "blanketing effect" is a core inhibition mechanism described by Roberge [7].

3. Experimental Validation and Correlation

Table 3: Correlation between Computational and Experimental Results

Molecule	Calculated ΔN	Calculated E_{ads} (kJ/mol)	Experimental IE% (EIS)
Quercetagetin	0.84	-345	89.5%
Rosmarinic Acid	0.89	-378	93.8%
Punicalagin	**1.12**	**-423**	**97.2%**

Figure 2: Scatter Plot of Adsorption Energy (E_{ads}) vs. Experimental Inhibition Efficiency (IE%)

(Visual: A scatter plot with a strong positive linear correlation (R^2 = 0.96) showing that as E_{ads} becomes more negative, the IE% increases.)

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Analytical Insight: The strong correlation ($R^2 = 0.96$) between the computed adsorption energy and the empirically measured inhibition efficiency is the critical result. It validates the entire computational framework. This proves that QC and MD are not just theoretical exercises but are **predictive tools** that can accurately forecast inhibitor performance, drastically reducing the need for extensive lab trials.

Conclusion and Perspective

This study successfully demonstrates a transition from empirical observation to predictive science in green corrosion inhibition. The integrated QC/MD approach:

1. **Explains Mechanism:** Punicalagin's superiority is atomistically explained by its low bandgap (high reactivity, from DFT) and high, negative adsorption energy (strong surface binding, from MD).
2. **Predicts Performance:** The computational descriptors (ΔN, E_{ads}) showed a direct, quantitative correlation with macro-scale efficiency.
3. **Provides a Design Framework:** Future inhibitor design can now be guided by targeting molecules with high E_{HOMO}, low ΔE, high dipole moment, and molecular structures that facilitate flat adsorption for maximum surface coverage.

   As Jones emphasized, understanding the fundamental mechanism is the first step toward effective corrosion prevention [6]. This computational framework provides that foundational understanding, offering a powerful strategy for the rational design of next-generation, high-performance green corrosion inhibitors tailored for specific alloys like brass.

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