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## Quantum Computing for Corrosion Simulation: Workflow and Resource Analysis

*Monday 1 December 2025 16:00 (1 hour)*

Corrosion is a pervasive issue that impacts the structural integrity and performance of materials across various industries, imposing a significant economic impact globally. In fields like aerospace and defense, developing corrosion-resistant materials is critical, but progress is often hindered by the complexities of material-environment interactions. While computational methods have advanced in designing corrosion inhibitors and corrosion-resistant materials, they fall short in understanding the fundamental corrosion mechanisms due to the highly correlated nature of the systems involved. This paper explores the potential of leveraging quantum computing to accelerate the design of corrosion inhibitors and corrosion-resistant materials, with a particular focus on magnesium and niobium alloys. We investigate the quantum computing resources required for high-fidelity electronic ground-state energy estimation (GSEE), which will be used in our hybrid classical-quantum workflow. Representative computational models for magnesium and niobium alloys show that 2292 to 38598 logical qubits and  $(1.04 \text{ to } 1962) \times 10^{13}$  T-gates are required for simulating the ground-state energy of these systems under the first quantization encoding using plane waves basis.

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