Preface

"There's Plenty of Room at the Bottom"
Richard P. Feynman

Catalysis has long been a cornerstone of chemical research, generating innovation across a wide range of sectors. Catalysts, by their very nature, accelerate chemical reactions, making them more efficient and sustainable. Over the last few decades, advances in nanotechnology have paved the way for innovative catalytic materials, with single-atom catalysts (SACs) emerging as a revolutionary class. My research on SACs is motivated by their extraordinary ability to change catalytic processes. Unlike conventional catalysts, SACs maximize the use of each atom, providing unparalleled activity and selectivity. This distinguishing feature not only promises improved performance but also adheres to the principles of green chemistry by reducing waste and energy consumption. The study of SACs is an important step in developing more efficient and ecologically friendly industrial processes. The relevance of this research goes beyond academic interest. SACs have a wide range of uses, including energy conversion, environmental remediation, and chemical synthesis. SACs, for example, could help to develop cleaner energy technologies by increasing the efficiency of fuel cells for hydrogen production. Similarly, in environmental applications, SACs may aid in the reduction of hazardous emissions and the efficient breakdown of contaminants. As a result, the findings of this thesis may help to address some of our society's most urgent issues.

Overall, the thesis is divided into six chapters, beginning with the notion of catalysis, its evolution, and the introduction of SACs in Chapter 1, and continuing with the theoretical framework and methodology utilized in the thesis in Chapter 2. In

Chapter 3, we addressed our research into cobalt (Co) SACs over Psi-graphene for the CO oxidation reaction. Chapter 4 discusses our research into the catalytic activity of nickel (Ni) SACs embedded on various substrates towards the hydrogen evolution reaction. In Chapter 5, we presented our findings on the catalytic performance of several transition metals (Ni, Pd, Pt, Cu, Ag, and Au) implanted in an AlN substrate for the water-gas shift process. Finally, we finish our thesis and reflect on prospects for the future.