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Examining the rudimentary steps of the oxygen reduction reaction on single-atomic Pt using Ti-based non-oxide supports

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In the attempt to reduce the high-cost and improve the overall durability of Pt-based electrocatalysts for the oxygen reduction reaction (ORR), density-functional theory (DFT) calculations have been performed to study the energetics of the elementary steps that occur during ORR on TiN(100)- and TiC(100)-supported single Pt atoms. The O_2 and OOH^* dissociation processes on Pt/TiN(100) are determined to be non-activated (i.e. "barrier-less" dissociation) while an activation energy barrier of 0.19 and 0.51 eV is found for these dissociation processes on Pt/TiC(100), respectively. Moreover, the series pathway (which is characterized by the stable OOH^* molecular intermediate) on Pt/TiC(100) is predicted to be more favorable than the direct pathway. Our electronic structure analysis supports a strong synergistic co-operative effect by these non-oxide supports (TiN and TiC) on the reduced state of the single-atom Pt catalyst, and directly influences the rudimentary ORR steps on these single-atom platinized supports.

I. INTRODUCTION

Amongst many oxygen-related (electro)chemical reactions, oxygen reduction reaction (ORR) [1–3] is one of the fundamentally important and technologically relevant reactions for many clean energy processes, e.g. hydrogen-based fuel cell technology [4]. Due to its generally low operating temperatures and overall light weight, the proton exchange membrane fuel cells (PEM FCs) are often considered as a suitable candidate for portable energy applications, such as hydrogen-fuel operated vehicles [5]. However, the overall efficiency of these PEM FCs are often plagued by the slow kinetics of the ORR, high cost of the platinum catalyst, and long-term durability issues [5, 6].

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