Getting the electrons right for O2-on-metal systems

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"My heart tells me that he has some part to play yet, for good or ill, before the end; and when that comes, the pity of Bilbo may rule the fate of many - yours not least."

J.R.R. Tolkien, *The Shadow of the Past - Fellowship of the Ring*, July 1954

"Don't worry about the future. Or worry, but know that worrying is as effective as trying to solve an algebra equation by chewing bubble gum. The real troubles in your life are apt to be things that never crossed your worried mind, the kind that blindside you at 4 pm on some idle Tuesday."

Mary Schmich, *Chicago Tribune*, June 1997.

Foreword

Before the start of this thesis, it might be useful to quickly go over its scope, aims and goals. The main goal of this thesis is to convey the new scientific work of the last four and a half years regarding the “difficult” molecule-metal systems, or put more specifically: O_2-on-metal systems. However, I would additionally like to use this thesis as an accessible way to cover some of the background of surface science and theoretical chemistry. I do this with the hope to make the new scientific content of Chapters 3-5 more accessible for those outside the field. Therefore, the first chapter is written in a way that I believe will be understandable for a broad audience, such that the general background of this thesis and the reasons for this work can be easily understood. Similarly, the second chapter has been somewhat extended beyond the scope commonly found in theses in this field. This is done to ensure that it forms a more complete picture of the methods and theories used in theoretical surface science. Either way, the first two chapters should form a solid context in which to place the other three scientific chapters. These three chapters are based on three scientific publications and will therefore be far more niche in their content and language. Now, with this out of the way, let’s get started.

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