Getting the electrons right for O2-on-metal systems

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Stellingen
Behorend bij het proefschift
Getting the electrons right for O_2-on-metal systems

i. Any future use of the non-self-consistent-field (NSCF) hybrid DFT approach will require a full self-consistent-field result for verification, reducing the effectiveness of the NSCF approach. *(Chapter 3)*

ii. The hole model presents a useful method to investigate the quality of a potential energy surface, as it samples all possible barriers to reaction. *(Chapter 3)*

iii. QCT dynamics calculations based on a BOSS DFT will not be able to achieve the radical changes in the potential energy surface of O_2 on Al(111) that are needed to resolve the shortcomings of current theoretical models. *(Chapter 4)*

iv. A highly accurate screened hybrid Van der Waals DF for O_2 + Cu(111) must exist, even though it has not yet been found. *(Chapter 5)*

v. The necessary study of O coverage dependencies for O_2 + metal interactions on the screened hybrid DFT level will remain difficult as long as the high computational demands associated with hybrid DFT cannot be resolved. *(M. M. Montemore, et. al., Chem. Rev., vol. 118, pp. 2816–2862, 2018*)

vi. Single minimum barriers should not be carelessly used to verify the accuracy of an entire potential energy surface for molecule metal interactions. Similarities in the DFT description of the energetic corrugation of the barrier are not always shared between different density functionals (DFs). *(M. Wijzenbroek and G. J. Kroes, J. Chem. Phys., vol. 140, p. 084702, 2014.)*

vii. The commonly applied measure for chemical accuracy (*1 kcal/mol*) is not useful when dealing with highly reactive chemical systems, namely, systems with reaction barriers of only a few *kcal/mol*. *(N. Gerrits, et. al., J. Phys. Chem. Lett., vol. 11, pp. 10552–10560, 2020)*

viii. The problem with the proliferation of different DFs in theoretical chemistry cannot be resolved. Any attempts to do so will only add more DFs and thus expand the problem. *(N. Mardirossian and M. Head-Gordon, Mol. Phys., vol. 115, pp. 2315–2372, 2017*; *M. Spiegel, et. al., Molecules, vol. 26, p. 5058, 2021)*

ix. The use of a sensible unit is instrumental for a good understanding of a value. For example, the value of a 'Twinkie' (*1 Twinkie≈140 kcal ≈ 3.6*10^{24} eV*) can be used in surface science but it gives little insight in the meaning of the energy values on the relevant surface science energy scale (*≈ 1 eV*). *(I. Reitman, United States. Ghostbusters, (1984))*

x. Het is opmerkelijk dat op een universiteit die zichzelf prijst als bolwerk van vrijheid de stellingen van promovendi getoetst moeten worden door leden uit twee hogere hiërarchische lagen. *(zie: Promotiereglement Universiteit Leiden 2024)*

xi. Het feit dat het aantal mensen met burn-out klachten de afgelopen tien jaar toegenomen is toont aan dat het verhaal van Rupsje Nooitgenoeg toch ook een ander einde kent. (*Nationale Enquête Arbeidsomstandigheden, CBS, TNO*)

xii. Onderschat nooit de waarde van een goede partij mokken.

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