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Characterisation of Sulphur oxide and water co-adsorption on Pt(111)

The recent movement towards renewable and sustainable sources of energy has received significant interest of late. Among others, solar, wind and hydrogen have been identified as viable alternatives for fossil fuels whereof the latter proposed alternative receiving particular attention. Among others, the HyS cycle serves as one process for the obtainment of hydrogen. Herein a metal catalyst, often being Pt due to its highly efficient catalytic properties, is employed to enhance the oxidation of SO_2 with H_2O [1]. Although experimental investigations concerning both adsorption and desorption of species, such as SO_2 and H_2O, on Pt surfaces have been reported, little is known regarding the interaction among these co-adsorbed species [2–4]. As a result, the charge interaction between various co-adsorbed species on Pt(111) was investigated through the use of density functional theory within the Vienna Ab Initio Simulation Package framework, employing 120 cores per calculation, at the Centre for High Performance Computing, South Africa [5,6].
It was observed that the charge interaction between sulphur oxides and the Pt(111) are stronger in all adsorption systems than the interaction between Pt(111) and H_2O. Through the employment of Bader Charge Analysis, it was noted that partial charge transfer between Pt and sulphur oxides are significantly greater than for charge transfer between Pt and H_2O. In addition to differences in charge transfer properties between Pt and different adsorbed species, are different susceptibilities for the respective adsorbates, in terms of energy as well as charge interaction with the metal surface observed when co-adsorption occurs.

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