

## **510g A Density Functional Model for Tuning the Charge Transfer between the Platinum Catalyst Electrode and Chemisorbed Species Via the Electrode Potential**

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A simple approach is proposed to predict the magnitude of charge transfer between a polarized transition metal electrode and a chemisorbed species (Oxygen/ Hydrogen) in an electrolytic solution. The approach is based on the equalization of the chemical potentials, as defined in density functional theory (DFT). The system is modeled using a platinum cluster representing the platinum electrode and a molecule. Electric field due to the electrical double layer (EDL) is simulated by either a set of point charges or an externally applied electric field of appropriate magnitude. The result of this research allows us to point out the various factors determining the nature of charge transfer in electrochemical reactions occurring in fuel cells, in particular those involving Oxygen (such as in Oxygen Reduction Reaction, ORR) or Hydrogen.