Electronic Study of Platinum/Graphite/Gases (CO, H₂, O₂) System

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Abstract

The objective of our research will be to study the interactions in a platinum/graphite catalyst used as an anode of a PEM fuel cell and its influence on reactions at a quantum level and scale it up to atomistic and molecular levels. The metal-metal, metal-support and gas-metal-support interaction can be described by ab initio quantum mechanics simulations. Information like partial charges, dipole moment, surface geometries, vibrational frequencies, energetics, etc., for a system can be obtained from the ab initio calculations, which can be incorporated into a more approximate molecular level simulation like Monte Carlo (MC). It will describe the atomic structure of a catalyst and its reactivity in a larger scale, close to macroscopic dimensions.