Fuel cell basics revisited: the migration of hydrogen on platinum

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Among alternatives to depleting fossil fuels being sought after across the globe, hydrogen has been seen as the most promising candidate due to its exemplary environmental compatibility and high utilization efficiency, in the company of several other advantages. Together with pressing economic factors, these potentials have inspired global moves towards the so-called hydrogen economy, marked by sweeping investments made in both public and private sectors in hopes of expediting an exit from current fossil-fuel based systems. It is however recognized that the task of a full shift to hydrogen systems has so far been and still is a daunting one, confronted with challenges in all aspects of its proposed daily application: production, storage, and practical utilization.

We focus on the latter aspect in this study. Knowledge on the migration of light interstitials, particularly hydrogen, on platinum is essential in taking full advantage of the catalytic capability of this metal as part of fuel cell electrodes. On this aspect of our group's fuel cell research thrust we continue our studies on the fundamental problem of hydrogen motion on Pt(111). Using a potential energy surface derived from density functional theory-based calculations involving a rigid, five-atomic layer-thick slab for modeling the catalyst substrate, higher energy states for the H-Pt system at 1/4 coverage show that the migration barrier may go as low as 0.03 eV. This followed from a three-dimensional picture of the first excited state wave function describing hydrogen motion showing considerable delocalization (see Fig. 1, plotted along a unit cell of the 111 face of Pt), in contrast to the highly localized ground state. For a more comprehensive picture we are pursuing pertinent dynamics calculations for hydrogen motion.

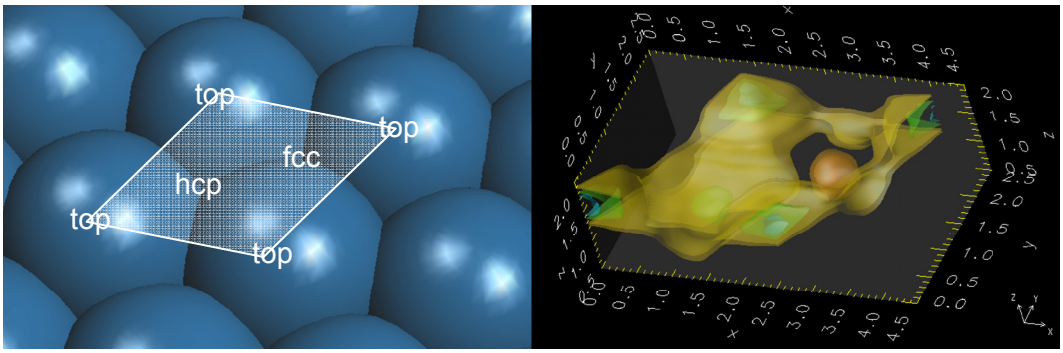

Fig. 1. The first excited state wave function, plotted on a surface primitive cell