

Abstract Submitted
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First principles studies of CO adsorption and diffusion over Pt nano-islands on Ru(0001) surface¹ SERGEY STOLBOV, University of Central Florida, MARISOL ANCANTARA ORTIGOZA, Kansas State University, TALAT S. RAHMAN, University of Central Florida — Proton exchange fuel cells are promising tools for hydrogen economy. However, CO, present in hydrogen, blocks active Pt sites of anode that poisons its reactivity. As reported [1], small coverage of Pt on Ru nanoparticles is much less sensitive to CO than commercial catalysts. To understand this effect, we have performed density functional theory based calculations of the energetics of adsorption and diffusion of CO on the 7Pt-atom islands and on the Ru(0001) substrate. We find that CO adsorption energy increases as it moves from the center of the Pt island to its edge and further onto substrate. CO thus tends to move from the Pt island to the Ru substrate. Diffusion barriers are found to be lower than 0.3 eV suggesting this process to be fast. This finding suggests that this hydrogen oxidation catalyst is CO tolerant because of the propensity of CO to move from active Pt island site to the Ru substrate. We present the rationale for this effect using insights from detailed electronic structure calculations. [1] S. R. Brankovic, et al., *Electrochem. Sol.-St. Lett.* **4** (12) A217-A220 (2001).

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