Abstract Submitted
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Formation of Pt nano-islands on Ru(0001) surface: insights from ab initio calculations .[1] TALAT S. RAHMAN, University of Central Florida, MARISOL ALCANTARA ORTIGOZA, Kansas State University, SERGEY STOLBOV, University of Central Florida — As reported [1], Ru nanoparticles with submonolayer of Pt are much more efficient catalysts for hydrogen oxidation than anodes used in standard fuel cells. Since this effect apparently depends on the size of Pt islands, we have performed density functional theory based calculations of energetics of Pt islands of varying size on the Ru(0001) surface. We find the formation energy of the island per atom to decrease monotonically from -5.1 eV to -6.1 eV, as the number of Pt atoms in the 2D island increases from one atom to one monolayer. Propensity of the systems to increase the number of interatomic bonds thus overpowers the effect of the stress caused by the 2.6% misfit of Ru and Pd interatomic bonds. As a result, Pt atoms prefer to coalesce on Ru(0001) increasing the cluster size up to one monolayer, in agreement with experimental data. This raises the question whether the key role of nano-sized Ru clusters [1] is to prevent coalescence of Pt islands by restricting their diffusion through facet edges. To address this issue we consider the effect of surface steps on Ru(0001) on the Pt island formation. 1. S. R. Brankovic, et al. , Electrochem. Sol.-St. Lett. **4** (12) A217-A220 (2001).

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