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**Pd/W(110) as a highly CO tolerant electrocatalyst for hydrogen oxidation: insight from first principles** NAGENDRA DHAKAL, SERGEY STOLBOV, University of Central Florida — Platinum perfectly catalyzes hydrogen oxidation reaction on the hydrogen fuel cell anodes. However, it has at least two drawbacks: a) it is too expensive; b) it has a low tolerance to CO poisoning. Pt-Ru bi-functional catalysts are more tolerant to CO, but they are still very expensive. In this work, we performed first-principle studies of stability reactivity of M/W(110) structures, where M=Pd,Ru,Au monolayers. All three systems are found to be stable: formation energy of MLs is significantly higher than cohesive energy of the M-elements. The calculated binding energies of H, $H_2$, OH, CO, and $H_2O$ were used to obtain the reaction free energies. Analysis of the free energies suggests that Au-W bonding does not activate sufficiently Au monolayer, whereas Ru/W(110) is still too reactive for the CO removal. Meanwhile, Pd/W(110) is found to catalyze hydrogen oxidation and at the same time to be highly tolerant to the CO poisoning. The latter finding is explained by the fact that CO binds much weaker to Pd on W(110) than to Pt, while the OH binding energy is strong enough to ensure CO oxidation. The obtained results are traced to the electronic structure of the systems.

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