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First principles studies of stability and reactivity of electro-catalysts for low-temperature fuel cells¹

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Low-temperature fuel cells (FC) are promising clean source of electric power. However, Pt-based catalysts make FC unacceptably expensive. Low rate of the oxygen reduction reaction (ORR) on the Pt cathode, and poisoning of anode by CO also reduce efficiency of FC. New materials such as Ru nanoparticles with the Pt (Pt/Ru) and Se (Se/Ru) sub-monolayer coverage demonstrate improved electro-catalytic activity (reactivity) towards anodic hydrogen oxidation and the cathode ORR, respectively. Pd-Co, CrN structures are also considered catalysts for ORR. Although reactivity is a key characteristic of the catalysts, their stability is also very important issue. The goal of this talk is to show the efficiency of the first principles computational approach to the problems of stability and reactivity of the electro-catalysts for FC. The stability problem is illustrated with our calculation results obtained for the Pt/Ru and Se/Ru nano-structures. By analyzing energetic and geometry of Pt and Se adsorption on Ru substrates, we find that Se and Pt atoms behave absolutely different on Ru: the Pt tend to join into large 1D islands, while Se atoms prefer to stay apart from each other on the substrate. The technique recently developed by Norskov group [1] is used in this work to evaluate the onset cathode potential for ORR on the Pd-Co, CrN and Se/Ru surfaces. We find a good agreement of the calculation results with available experiment. The power of computational methods also illustrated with the results explaining high tolerance of Pt/Ru nano-structures towards CO poisoning of the FC anode.

[1] J. K. Nørskov, et al., *J. Phys. Chem. B* 108, 17886 (2004).

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