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Stabilizing and enhancing activity of Ag as a catalyst for oxygen redaction reaction on hydrogen fuel cell cathodes[1] SERGEY STOLBOV, MARISOL ALCANTARA ORTIGOZA, University of Central Florida — Progress in searching for cost-effective and highly active catalysts for the oxygen reduction reaction (ORR) on hydrogen fuel cell cathodes is hindered by the fact that only a few elements (expensive and scarce Pt, Ir, Au) do not dissolve in the reaction environment (acidic medium at the expected operating potential +0.8 to +1.0 V vs SHE). Yet, in this work, we explore silver as an active element for the ORR catalysts. Although the dissolution potential (DP) of elemental Ag is 0.8 V, we rely on our finding [1] that binding of a metal monolayer (ML) to a reactive substrate can significantly increase its DP. Using our approach [1], we select Ag/Ru/W, Ag/Nb, and Ag/Ta as promising candidates for the ORR catalysts (where Ag and Ru are MLs). Our evaluation of DP within density functional theory (DFT) shows that, indeed, in the selected structures, DP of Ag significantly increases as compared to that of Ag(111) and, in the case of Ag/Nb, even exceeds that of Pt. The ORR free-energy diagrams calculated within DFT suggest that the above systems are more active toward ORR than Pt. We thus predict here three highly active and truly cost-effective ORR catalysts. [1] S. Stolbov, M. Alcantara Ortigoza, J. Phys. Chem. Letts. 3, 463 (2012).

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Sergey Stolbov
University of Central Florida

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