Composition-Activity-Stability Relationship in Bimetallic Pt-Au Oxygen Reduction Reaction Catalyst

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According to the recently announced Green Deal, hydrogen-fueled proton-exchange membrane fuel cells (PEMFCs) are expected to become one of the pillars of a future sustainable green-energy system. To date, the main limitations hindering the vast commercialization of such fuel cells reside on its cathode side, where a sluggish oxygen reduction reaction (ORR) takes place [1]. Because of that, PEMFC cathode requires a large amount of expensive platinum catalyst, which moreover operates under an aggressive corrosive environment. Therefore, recent research efforts have been focused on improving cost-efficiency and/or stability of ORR catalysts. While the majority of studies focus on improving cost-efficiency of platinum catalyst by preparing various platinum-based alloys [2], significantly less attention is devoted to improving its stability.

Herein, we report a study of Pt–Au alloys with different compositions (Pt₉₅Au₀₅, Pt₉₀Au₁₀, Pt₈₀Au₂₀) prepared using a magnetron sputtering technique [3]. The promising stability improvement of the Pt–Au catalysts, manifested in suppressed Pt dissolution with increasing Au content, was documented over an extended potential range up to 1.5 V_{RHE}. On the other hand, at elevated concentrations, Au showed a detrimental effect on ORR activity. A systematic study involving complementary characterization techniques, electrochemistry, and Monte Carlo simulations based on density functional theory data enabled us to gain a comprehensive understanding of the composition–activity–stability relationship to find an optimal Pt–Au alloying for maintaining the activity of platinum and improving its resistance to dissolution. According to the results, Pt–Au alloy with 10% gold represents the most promising composition retaining the activity of monometallic Pt while suppressing Pt dissolution by 50 % at the upper potential limit of 1.2 V_{RHE} and by 20 % at devastating 1.5 V_{RHE}.

The work was financially supported the Czech Science Foundation, project No. 22-03643S.

I. Khalakhan, ACS Appl. Mater. Interfaces, 15, 1192 (2023)

^[1] J. K. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J.R. Kitchin, T. Bligaard, H. Jónsson, J. Phys. Chem. B, 108, 17886 (2004)

^[2] L. Huang, S. Zaman, X. Tian, Z. Wang, W. Fang, B.Y. Xia, Acc. Chem. Res., 54, 311 (2021)

^[3] X. Xie, V. Briega-Martos, R. Farris, M. Vorokhta, M. Dopita, T. Skála, I. Matolínová, K.M. Neyman, S. Cherevko,