510f Thermodynamic Guidelines for Determining Efficient Oxygen-Reduction Catalysts

Perla B. Balbuena, Yixuan Wang, Sergio R. Calvo, Luis A. Agapito, Liuming Yan, and Jorge M. Seminario

Thermodynamic analyses of the individual reaction steps for oxygen reduction on transition metal catalysts permit to identify suitable combinations of elements which facilitate the overall oxygen reduction reaction. We discuss the methodology and the predictions obtained for a series of systems, some of them (such as Pt3Co, and Pt3Ni) already found experimentally.