

Abstract Submitted
for the DAMOP15 Meeting of
The American Physical Society

Tunable Catalysis of Water to Peroxide with Anionic, Cationic, and Neutral Atomic Au, Ag, Pd, Rh, and Os¹ K. SUGGS, F. KIROS, A. TESFAMICHAEL, Z. FELFLI, A.Z. MSEZANE, Clark Atlanta University — Fundamental anionic, cationic, and neutral atomic metal predictions utilizing density functional theory calculations validate the recent discovery identifying the interplay between Regge resonances and Ramsauer–Townsend minima obtained through complex angular momentum analysis as the fundamental atomic mechanism underlying nanoscale catalysis. Here we investigate the optimization of the catalytic behavior of Au, Ag, Pd, Rh, and Os atomic systems via polarization effects and conclude that anionic atomic systems are optimal and therefore ideal for catalyzing the oxidation of water to peroxide, with anionic Os being the best candidate. The discovery that cationic systems increase the transition energy barrier in the synthesis of peroxide could be important as inhibitors in controlling and regulating catalysis. These findings usher in a fundamental and comprehensive atomic theoretical framework for the generation of tunable catalytic systems. The ultimate aim is to design giant atomic catalysts and sensors, in the context of the recently synthesized tri-metal Ag@Au@Pt [1] and bimetal Ag@Au [2] nanoparticles for greatly enhanced plasmonic properties and improved chemical stability for chemical and biological sensing.

[1] N. Deogratias, M. Ji, Y. Zhang, J. Liu, J. Zhang and H. Zhu, *Nano Res.* **8**(1), 271 (2015)

[2] Y. Yang, J. Liu, Z.-W. Fu, and D. Qin, *J. Am. Chem. Soc.* **136**, 8153 (2014)

¹Research was supported by U.S. DOE Office of Basic Energy Sciences

Zineb Felfli
Clark Atlanta University

Date submitted: 29 Jan 2015

Electronic form version 1.4