

Abstract Submitted
for the DAMOP12 Meeting of
The American Physical Society

Atomic Au and Pd Negative-Ion Catalysis of H₂O, HDO, and D₂O to Corresponding Peroxides¹ ARON TESHAMICHAEL, KELVIN SUGGS, ZINEB FELFLI, XIAO-QIAN WANG, ALFRED Z. MSEZANE, Clark Atlanta University — Fundamental ideas of muon-catalyzed fusion utilizing a negative muon, a deuteron and/or a triton, have been used in atomic Au and Pd negative ion-catalysis of H₂O₂, HDO₂, and D₂O₂ from H₂O, HDO, and D₂O, respectively, finding that Au⁻ is an excellent catalyst but the Pd⁻ ion has a higher catalytic effect, consistent with recent observations. The fundamental atomic mechanism responsible for the oxidation of water to peroxide has been attributed to the interplay between Regge resonances and Ramsauer-Townsend minima in low energy electron elastic total cross sections for Au and Pd atoms, along with their large electron affinities. Dispersion-corrected density-functional theory transition state calculations performed on atomic Au⁻ catalysis of water conversion to H₂O₂, have revealed that the formation of the Au⁻(H₂O)₂ anion molecular complex in the transition state, provides the fundamental mechanism for breaking the hydrogen bonding strength in the catalysis of H₂O₂ using the Au⁻ ion. Thus, the crucial link between low-energy electron elastic scattering resonances and low-energy chemical reaction dynamics has now been fully established.

¹Research supported by DOE Office of Science; AFOSR and Army Research Office

Zineb Felfli
Clark Atlanta University

Date submitted: 25 Jan 2012

Electronic form version 1.4