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Charge modification of metal atoms: Catalysis of Water to Peroxide

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Synopsis Here we investigate the optimization of the catalytic behavior of Au, Ag, Pd, Rh, and Os atomic systems via charge modification 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. This conclusion should also be applicable to the oxidation of methane to methanol without CO₂ emission, with the anionic Os being the best catalyst.

In [1] it was demonstrated that the fundamental mechanism of negative ion catalysis of water to peroxide using atomic Au⁻ is the formation of the anionic Au⁻(H₂O)_{1,2} molecular complex during the transition state, which breaks up the H-O bonds, thereby promoting the formation of the H₂O₂ in the presence of O₂. The relatively large electron affinity (EA) of Au contributes to its anionic catalytic effectiveness. Our complex angular momentum (CAM) method [2] has been used to select the above metal atoms through the accurate determination of their large EAs for the investigations. Density Functional Theory (DFT) and dispersion corrected DFT approaches have been employed for the transition state

calculations. Geometry optimization of the structural molecular conformation utilized the gradient-corrected Perdew-Burke-Ernzerhof parameterizations [3] of the exchange-correlation as implemented in DMol3 [4]. A tolerance of 1x10⁻³ Ha was used with a smearing value of 0.005Ha.

Transition state calculated results, given in Fig. 1 show the catalyzing effects of cationic, neutral, and anionic Ag, Au, Pd, Rh, and Os atoms when synthesizing water to peroxide. Clearly, the Au⁺ is the least efficient of the given systems as shown by a barrier of ~1.3eV. Conversely, Os⁻ is energetically the most favored with a barrier of ~0.16eV as shown in Fig. 1(b).

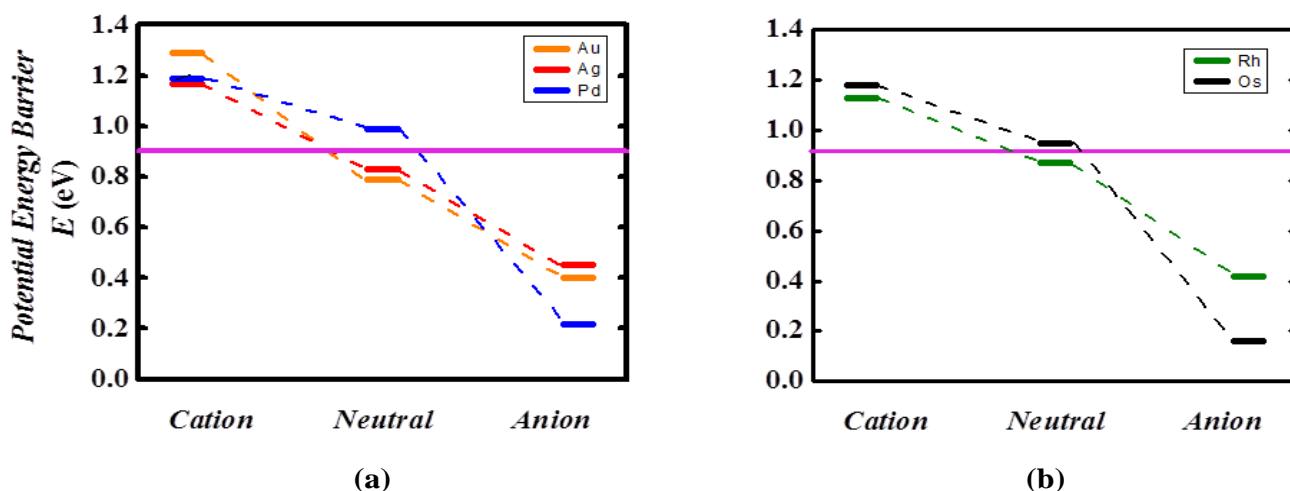


Figure 1 (a) and (b): Potential energy transition state barrier calculations of cationic, neutral, and anionic Au, Ag, and Pd and Rh, and Os represented by orange, red, and blue and olive and black, respectively. The standard comparative reaction energy without catalysis is represented by the purple line.

The discovery that cationic systems increase the transition energy barrier in the synthesis of peroxide could render them 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. We conclude that anionic atomic systems are optimal for catalyzing the oxidation of water to peroxide, with Os⁻ being the preferred candidate among the atomic ions proposed in this work. Whether this is consistent across interdisciplinary systems, reaction types, and atomic cluster substrates is yet to be determined.

The structure and dynamics of these atoms with relatively large EAs will facilitate the understanding of the recently synthesized Ag@Au@Pt nanosystem [5] with greatly enhanced plasmonic properties as well as lead to the creation of tunable supercatalysts.

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