

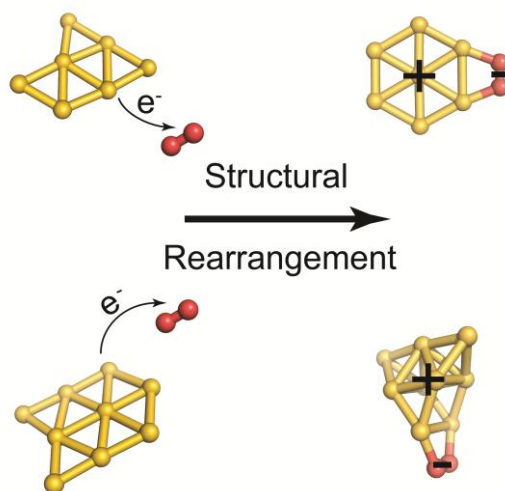
Oxygen binding and activation by anionic, neutral and cationic gold clusters

Alex P. Woodham^{1,2}, Gerard Meijer¹, André Fielicke²

¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

²Institut für Optik und Atomare Physik, Hardenbergstr. 36, 10623 Berlin, Germany
woodham@fhi-berlin.mpg.de

Gold remains one of the most prominent examples of the novel chemical and physical properties materials gain upon entering the nano-size regime. The now famous catalytic chemistry of gold in this size range starkly contrasts with the, equally well known, nobility of the bulk matter. The origin of this catalytic activity of gold nano-particles, and the mechanism by which they can activate molecular oxygen, remains an open question at the forefront of cluster science. We present here an Infrared Multiple Photon Dissociation (IR-MPD) investigation into the $Au_n(O_2)_m^{-/0/+}$ ($n=2-21$; $m=1-4$) complexes. By measuring IR spectra in the range of the O-O stretching vibrations of the different oxygen charge states (Superoxo (O_2^-); 1090 cm^{-1} , Physisorbed (O_2^0); 1580 cm^{-1} , and Dioxygenyl (O_2^+); 1900 cm^{-1}) we are able to ascertain the extent of charge transfer to and from the gold clusters and thus gain insights into the binding mechanisms responsible for oxygen activation. Comparison with quantum chemical calculations reveals that these charge transfer processes are mediated by structural rearrangement of the core cluster structure.



References:

- [1] A. P. Woodham, G. Meijer, A. Fielicke, *Angew. Chem. Int. Ed.* **51**, 4444-4447 (2012).
- [2] A. P. Woodham, G. Meijer, A. Fielicke, *J. Am. Chem. Soc.* **135**, 1727-1730 (2013).