Search Directions for Direct H2O2 Synthesis Catalysts Starting from Au-12 Nanoclusters - DTU Orbit (23/12/2018)

**Search Directions for Direct H2O2 Synthesis Catalysts Starting from Au-12 Nanoclusters**

We present density functional theory calculations on the direct synthesis of H2O2 from H-2 and O-2 over an Au-12 corner model of a gold nanoparticle. We first show a simple route for the direct formation of H2O2 over a gold nanocatalyst, by studying the energetics of 20 possible elementary reactions involved in the oxidation of H-2 by O-2. The unwanted side reaction to H2O is also considered. Next we evaluate the degree of catalyst control and address the factors controlling the activity and the selectivity. By combining well-known energy scaling relations with microkinetic modeling, we show that the rate of H2O2 and H2O formation can be determined from a single descriptor, namely, the binding energy of oxygen (E-O).

Our model predicts the search direction starting from an Au-12 nanocluster for an optimal catalyst in terms of activity and selectivity for direct H2O2 synthesis. Taking also stability considerations into account, we find that binary Au-Pd and Au-Ag alloys are most suited for this reaction.

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