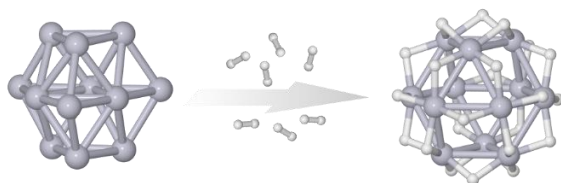


Pt₁₂H₂₄⁻: A Cuboctahedral Platinum Hydride Cluster Cage

Siddhi Gojare¹, Dennis Bumüller¹, Stephan Kohaut¹, Manuel Kraft¹, Detlef Schooss¹, Karin Fink¹

¹ Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany

E-Mail presenting author: siddhi.gojare@kit.edu



The heterogeneous catalysts consisting of Pt-nanoclusters supported on metal oxide surface exhibit quite versatile catalytic properties and are widely applied in automotive

catalytic converters, in the catalytic oxidation and reduction reactions, and for emission control [1]. Such nanoclusters have high catalytic activity and show diversity in a small energy range. A thorough study of the gas-phase cluster structure is needed to understand the underlying mechanisms of the surface reactions. In the current study, we combined trapped ion electron diffraction with density functional theory to analyze the effect of hydrogen on the Pt₁₂⁻ structure in the gas phase. The results showed that spin-orbit coupling did not influence the structures and the energetic ordering of the Pt₁₂H₂₄⁻ isomers. Among all the isomers, the isomer having a cuboctahedral cage structure was found to be most stable irrespective of the low coordination number of the Pt atoms. The structural analysis revealed that bridge-bound hydrogen atoms stabilize the structure through strong interactions with the neighboring Pt atoms by multi-center bonds resulting in higher charge transfer and thus high binding energy. The electronic effects show the presence of all-metal aromaticity.

[1] Kerpál C. et. al. J. Phys. Chem. A 2013, 117, 1233-1239.

[2] Siddhi Gojare, Dennis Bumüller, Stephan Kohaut, Manuel Kraft, Karin Fink, Detlef Schooss, Pt₁₂H₂₄⁻: A Cuboctahedral Platinum Hydride Cluster Cage, ChemPhysChem – Manuscript submitted