

Computational Study of Gold Nanoparticles

Hadi Abroshan and Hyung J. Kim

Carnegie Mellon University, Department of Chemistry, Pittsburgh 15213 PA

Abstract

Nanoparticles are at the leading edge of the rapidly growing field of nanotechnology with a wide range of applications such as nanocatalysis, sensing, photovoltaics, biology, etc. Atomic level understanding of nanoparticles' structure is of great importance to establish definitive structure–activity relationships in that it facilitates systematic development and applications of nanoparticles. In this regard, atomically precise gold nanoclusters have attracted great interest over the last decade from basic research to technological applications. In the study presented here, computational methods are applied to obtain fundamental understanding of optical and catalytic properties of atomically well-defined Au₂₅ clusters and their variants. Examples include the catalytic activity of nanoclusters in the hydrogenation of aldehydes as well as in the Ullmann and the Suzuki coupling reactions.