学术报告

报告题目： **Catalysis Application of Gold Nanoclusters**

报 告 人： 李 杲 副研究员（所百人，青千候选人）

报告时间： **2014年10月17日（周五）下午3：30**

报告地点： **固体所小楼312会议室**

报告摘要：

Recently, Gold complexes and nanoclusters have shown great promise as catalysts for carbon-carbon reactions. Herein, we have exploited the $Au_{25}(SR)_{18}$ gold nanoclusters as effective heterogeneous catalysts for Ullmann homo-coupling and Songashira cross-coupling reactions. The $Au_{25}(SR)_{18}$ nanoclusters were directly deposited onto various oxide supports (e.g., TiO_2, CeO_2, SiO_2 and Al_2O_3) and annealed at 150^{o}C in a vacuum, and these $Au_{25}(SR)_{18}$/oxide catalysts were then evaluated for the Ullmann-type homo-coupling and Songashira cross-coupling reaction. The oxide-supported $Au_{25}(SR)_{18}$ nanoclusters gave rise to very high conversions of iodobenzene (up to 99.8% with $Au_{25}(SR)_{18}/CeO_2$ catayst), and it also showed excellent catalytic actives for a variety of aryl iodides in Ullmann-type homo-coupling. On the other hand, the $Au_{25}(SR)_{18}/CeO_2$ catalyst also gave rise to high conversion of *p*-iodoanisole (up to 96.1%) and excellent selectivity for the target cross-coupling product (up to 88.1%) in the Songashira cross-coupling of *p*-iodoanisole and phenylacetylene. The oxide-supported $Au_{25}(SR)_{18}$ nanocluster catalysts showed excellent recyclability in the both C-C coupling reactions.

The density functional theory showed that adsorption energy of the iodobenzene and phenylacetylene were -0.40 and -0.48 eV, and of the co-adsorption was -0.90 eV. And it also found that iodobenzene and phenylacetylene were absorbed on different gold atoms, and pointed toward to the third gold atom together, which implied that the facets of the $Au_{25}(SR)_{18}$ clusters (comprised three surface gold atoms) should be the catalytic active cites of the C–C coupling reactions.

报告人简介:

学士 (2004): 湖南师范大学

博士 (2011): 上海交通大学

博士后(2011-2014): 卡内基梅隆大学

副研究员(2014-): 大连化学物理研究所催化国家重点实验室金催化中心

主要研究领域: 金纳米催化