乞
研究室内掲示

# 第 46 回 理学部化学科コロキウムの御案内

## "Computational Studies of Nanoalloys; Structures, Stabilities and Segregation in Bimetallic Clusters"

**Dr. Roy L. JOHNSTON**

School of Chemistry, University of Birmingham

日時：2004 年 10 月 20 日（水曜日）16：00～17：00

場所：国際交流会館・中会議室

**Abstract:** The desire to fabricate materials with well defined, controllable properties and structures, on the nanometre scale, coupled with the flexibility afforded by intermetallic materials, has generated interest in bimetallic alloy clusters or "nanoalloys". One of the major reasons for interest in nanoalloy particles is the fact that their chemical and physical properties may be tuned by varying the composition and atomic ordering, as well as the size of the clusters. Their surface structures, compositions and segregation properties are of interest as they are important in determining chemical reactivity, and especially catalytic activity. Nanoalloy clusters are also of interest as they may display structures and properties which are distinct from those of the pure elemental clusters.

In this talk, I will start by introducing the field of nanoalloys in general and reasons for studying them. I will then describe the model (the Gupta many-body potential) and the methodologies (Genetic Algorithms and systematic optimization studies of geometric shell clusters) that we have used to study the structures and segregation properties of Cu-Au, Ag-Au, Ni-Al and Pd-Pt nanoalloys. I will conclude by summarizing the important factors that determine the mixing or segregation properties of nanoalloy clusters.

連絡先 橋本健朗（内線 2621）