Nano-space Function Design Seminar

14:30–16:30, July 14th (2017)

Common seminar room (2C5/2C7)

Discerning the Molecular in the Metallic: How Iterating Theory and Experiment Reveals Lessons for Materials Design in Complex Intermetallics

Prof. Daniel C. Fredrickson, Department of Chemistry, University of Wisconsin–Madison

Intermetallic phases—solid state compounds that form upon alloying metallic elements together—comprise a realm of immense structural diversity: their structures range from simple variants of the familiar *fcc*, *bcc* and *hcp* lattices, to the giant cubic unit cells of $NaCd_2$ (>1,000 atoms/cell) and $Al_{55.4}Cu_{5.4}Ta_{3.9}$ (23,134 atoms/cell), to quasicrystals such as $YbCd_{5.7}$ whose geometries defy description with 3-dimensional unit cells. A limiting factor in realizing the broad technological applications promised by this diversity of atomic arrangements is our inability to understand, let alone control, the crystal structures of these compounds. The goal of our research group is to determine the driving forces that underlie this diverse structural chemistry and, ultimately, to harness these forces in the design of new materials. Our approach is to iterate theoretical and experimental investigations into these compounds, such that new theoretical concepts inspire new synthetic endeavors and vice versa. In this seminar, we will discuss two connections to molecular chemistry that have emerged from this approach: (1) the role of simple molecular orbital schemes in defining the preferred electron counts of intermetallics, and (2) the prominence of conflicts between electronics and sterics in shaping intermetallic structures.

Electron counting in aluminum–transition-metal quasicrystals and related crystals

Koichi Kitahara, Department of Advanced Materials Science, the University of Tokyo

In 2014, essentially the same simple electron-counting scheme for main group–transition metal intermetallic compounds, now referred to as $18-n$ rule, was independently discovered by *the two research groups*. Now the scheme has successfully been applied to hundreds of intermetallic phases as is, but, in some cases, we needed to modify it. Such requirements are keys to notice a new concept. Our first target was the simplest quasicrystalline approximant in Al–Cu–Ir system. The scheme we actually found was not the $18-n$ rule, but we required a general variant of it. Recently, we extrapolated our understanding on the approximant to quasicrystals, where we found a possible further extension of the scheme.

References: Gordon G. C. Peterson, Vincent J. Yannello, and Daniel C. Fredrickson, Angew. Chem., Int. Ed. **56** (2017), in press (DOI: 10.1002/anie.201702156), and references therein. K. Kitahara and K. Kimura, Z. Kristallogr.—Cryst. Mater. (2017), in press (DOI: 10.1515/zkri-2016-2035), and references therein.