Molecular Geochemistry as a Basis for a Systematic Understanding of Environmental Behaviors of Various Elements

YOSHIO TAKAHASHI[1]

[1]The University of Tokyo, Tokyo 113-0033, Japan (*correspondence: ytakaha@eps.s.u-tokyo.ac.jp)

There are many emerging inorganic and organic contaminants in environment related to the development of new technologies. For exampe, the number of researches on Sb, Te, Tl, REE, and PGE has been increasing to deal with the emerging problems in terms of inorganic contaminants. It is possible that human beings must face unexpectedly with such new environmental problems caused by such elements. Thus, it is necessary for us to know systemtically all the elements. A systematic understandning gained through such researches on the various elements will enable us to predict environmental behaviors of any emerging elements.

For this purpose, understanding of the chemical species in natural systems and chemical processes from molecular-scale information is important. For example, adsorption at the solid-water interface is an important reaction during the migraiton of metal ions. In particular, formation of either inner- or outer-sphere complex at the solid-water interface is critial, which controls the distribution and even isotopic fractionation of trace elements. For this examplie, pKa or hydrolysis constant can be used to predict systematically the structure of surface complex and their distribution and isotope fractionation for oxyanions and cations, respectively.

X-ray absorption spectroscopy (XAS) has been an essential tool in this field. The atomic-scale information for varoius elements provided by the method coupled with quantium chemical calulation and various thermodynamic modelings allows us to clarify their atomic-scale interactions. Although normal fluorescence XAFS can beuseful for trace elements, wavelength dispersive XAFS can be poweful to detect elements at lower abundances. Interactions with organic matter and bacteria affect migration of trace elements through complexation, organigification, etc. The inorganic-organic interaction can be studied by XAS at soft X-ray region such as by scanning transmission X-ray microsocpy.

Professor V. M. Goldschmidt tried to understand distributions of all elements in varoius systems in the earth through phsyco-chemical knowledge. Today, we can get the actual atomic-scale information of trace elements, which he had to imagine at that time. In this recpect, this is the time to develop molecular geochemistry, which can be a basis to predict behaviors of any elements on the periodic table.