Novel Properties of Correlated Electrons in Alkali-Metal Clusters Incorporated in Regular Nanospace of Zeolite Crystals

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Abstract: Zeolites are porous crystals with the regular nanospace of cages. Guest alkali metals can be loaded into cages at various densities. Alkali-metal clusters are generated in cages together with zeolite cations. The transfer of *s*-electrons to adjacent clusters is provided through the windows of cages, which leads to an energy band of 3-dimensional cluster array. The Coulomb repulsion energy of *s*-electrons in cluster is large enough to have a strong electron correlation. Novel electronic properties, such as ferromagnetism, ferrimagnetism and antiferromagnetism, have been observed depending on the loading density of alkali metals, the structure of zeolite framework and the kind of alkali metals.

Aluminosilicate zeolite A has the negatively-charged framework with an LTA-type structure, where α-cages with an effective inside diameter of 11 Å are arrayed in a simple cubic structure. Potassium metal is loaded into K-type zeolite A ($K_{12}Al_{12}Si_{12}O_{48}$) at the average loading-density of K atoms, n, per α-cage, namely $K_{12+n}Al_{12}Si_{12}O_{48}$. With increasing n, *s*-electrons can occupy the 1*p*-like quantum state which is given by the spherical quantum-well model. We have observed ferromagnetic properties for $n > 2$. They are assigned to a canted antiferromagnetism, where canting angle may be strongly enhanced by the Dzyaloshinsky-Moriya interaction in the degenerate 1*p*-like states. Electric state is in a Mott insulator.

The framework of low-silica X (LSX) zeolite has an FAU-type structure, as shown in Fig. 1. Supercages and β-cages with respective inside diameters of 13 and 7 Å are arrayed in a diamond structure. In K-Na alloy clusters, a Néel's N-type ferrimagnetism has been observed at $n \approx 7.5$. Much higher values of n can be realized by the pressure loading of alkali metal, and ferromagnetic properties reappear at a certain loading pressure.

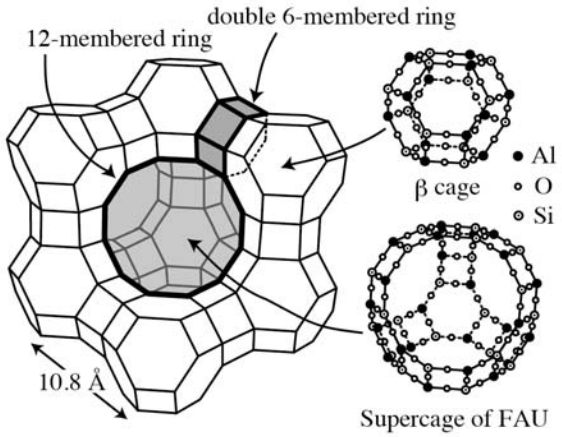

Fig. 1 Framework structure of low-silica X (LSX) zeolite. Cations are not shown here.

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