9. Multiplet Structures in $3d$ and $4d$ X-ray Core Photoemission Spectra for La and Ce Compounds

今田　真

Core-level spectroscopy is well known to be a very powerful tool to investigate electronic states in solids. In X-ray core photoemission, the response of outer electronic systems, both localized and itinerant, to the core hole produced by the incident photon is reflected in structures of the spectra.

We study $3d$ and $4d$ X-ray core photoemission spectra (XPS) for La and Ce compounds on the basis of the Anderson model which considers the hybridization between $4f$ states and valence band states. We concentrate on the multiplet structures arising from the interactions between $4f$ electrons and core hole. Narrowing of the multiplet structures occurs when the multiplets strongly mix with each other through the hybridization, while the multiplet structures are preserved when a sufficient mixing does not occur. We also attempt a consistent explanation of $3d$- and $4d$-XPS for each compound choosing reasonable parameters.

10. Pairing Mechanism of Holes in High Tc Superconductors —Attraction through spin polarization in the Cu-O plane—

西野友年

Excess holes in oxide superconductors which are responsible for superconductivity will enter hybridized orbitals between Cu $d_{3z^2-r^2}$ orbitals in the Cu-O plane and oxygen p_z orbitals in the Ba-O plane, if the Hund rule coupling in Cu-$3d$ orbitals is dominant. Then the excess holes itinerate among these orbitals. Since transfer of holes between Cu $d_{x^2-y^2}$ orbitals is suppressed by large intraatomic coulomb energy. The holes behave as local spins. We, therefore, represent the Cu-O plane by an antiferromagnetic Heisemberg spin system. There is a ferromagnetic interaction between the spin system and an excess hole caused by the Hund rule coupling within the

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Cu-3*d* orbitals. The excess holes polarize the spin system through this effect, thereby interacting among themselves through this polarization. Binding energy between two holes is calculated from the ground state energy of some finite size systems. The interaction is attractive in some parameter region where 2 holes make a singlet pair.

11. 遷移金属と軽い原子との合金の電子状態と磁性

山崎　亨

新しい永久磁石の素材である$Nd_2Fe_{14}B$において，ホウ素は強磁性を安定化するのにある役割を果たしていると考えられるが，完全に解明されているとはいえない。そして，B，C，Nなどの軽い元素が鉄の強磁性に及ぼす影響も，いまのところでは，1ケの不純物原子の場合にのみ報告されている。そこで，それらの原子を有限濃度含んだ置換型合金を考え，KKR－CPA－LSDにより電子構造を第一原理から計算し，それらの元素の合金効果を調べた。

12. A Temperature Shift Method in Canonical Molecular Dynamics

大塚博巳

We propose a method for obtaining the average values of physical quantities at temperatures different from the assumed value from a simulation calculation of the canstant temperature molecular dynamics (MD) with a fixed temperature. The method is developed on the basis of Nosé's canonical MD. The present method is numerically tested in a simulation on a 13-atom Lennard-Jones cluster.