Title

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

Author(s)

西野 友年

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

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

Excess holes in oxide superconductors which are responsible for superconductivity will enter hybridized orbitals between Cu \(d_{xz}\) 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 \(\text{Cu} d_{xz}\) 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
Cu-$3d$ 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. 還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$_2$Fe$_{14}$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 博己

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 constant 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.