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Pr sf effective exchange interaction and superconductivity in $PrOs_4Sb_{12}$

M. Koga[1], M. Matsumoto[2], H. Shiba[3], O. Sakai[4]

[1]Faculty of Education, Shizuoka University, Shizuoka, 422-8529
[2]Faculty of Science, Shizuoka University, Shizuoka, 422-8529
[3]Physical Society of Japan, Minato-ku, 105-0004
[4]Graduate School of Science, Tokyo Metropolitan University, Hachioji, 192-0397

The Pr skutterudites PrT_4X_{12} have many properties varied by changing the combination of transition-metal ions (T=Fe, Ru, Os) and pnictogens (X=P, As, Sb). Each Pr ion is located in a cage X_{12}, which leads to strong hybridization of Pr f-electron states with conduction bands. As a result, the complex structure of the Pr states in the f^2 configuration displays orbital ordering, multipolar effects and exotic metallic behavior.

It is known that $PrOs_4Sb_{12}$ is a heavy-fermion supercondoctor with broken time-reversal symmetry[1]. In a magnetic field, a multiple superconducting phase is reported[2]. An ordered phase is induced by a higher magnetic field in which the superconductivity disappears although a magnetic moment is absent at zero field[3]. The purpose of our study is to clarify the f-orbital nature of Pr ions in this physics.

Using our previous approach to U dilute alloys[4], we derive an sf effective exchange interaction for low-lying crystal-field states of Pr, considering T_h symmetry as the point group[5]. We choose a plausible level scheme in which the ground state is a Γ_1 singlet and the first excited state is a $\Gamma_4^{(2)}$ triplet[3]. We take into account a strongly hybridized a_u conduction band and some relevant t_u bands from molecular orbitals of Sb_{12}[6]. Within the a_u band, we obtain a magnetic exchange interaction only due to the Pr triplet. We have recently reported a possibility of exciton-mediated superconductivity based on this sf interaction[7]. Through the sf exchange, the low-lying excitations (excitons) with a finite energy gap give rise to an attractive interaction for Cooper pairing. The symmetry of the superconducting order parameter is determined by dispersion relation of the exciton. We find that a d-wave state ($k_xk_y+\omega k_yk_z+\omega^2k_zk_x$, $\omega = e^{\pm i2\pi/3}$) is stabilized for the bcc system $PrOs_4Sb_{12}$. This state breaks time-reversal symmetry.

For coupling of the Pr singlet and triplet states, the admixture of the a_u and t_u bands is necessary. This gives quadrupolar exchange as well as magnetic in the sf interaction, which should be important for understanding of the field-induced order. We generalize our theory including this exchange model.

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