PC2-1-INV

Superconductivity in layered tin pnictides with a van der Waals-type structure

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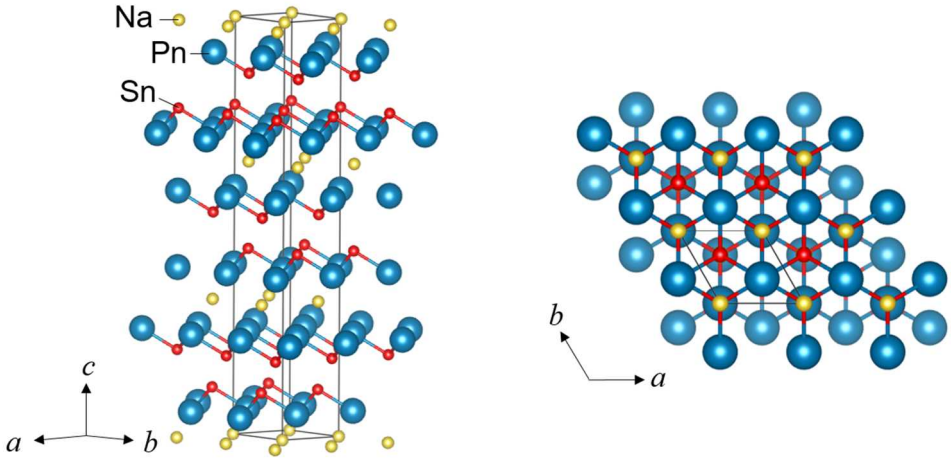
A layered crystal structure is an attractive stage to explore superconductors with a high transition temperature (T_c) and to discuss the mechanisms of unconventional superconductivity, as exemplified by the cuprates and the Fe-based superconductors. The discovery of a basic structure, which works as a superconducting layer, such as the CuO_2 plane and the Fe_2An_2 (An = P, As, S, Se, Te) layer, have opened new physics and chemistry fields on low-dimensional superconductors because many structural analogous could be designed by changing the structure or the alignment of the spacer layers as well as superconducting layers.
Recently, we reported SnPn-based (Pn: pnictogen) layered compounds $NaSn_2As_2$ and $Na_{1-x}Sn_2P_2$ [1,2] as a new class of van der Waals (vdW)-type superconductors. The crystal structure of these compounds is characterized by two layers of a buckled honeycomb network of SnPn, bound by the vdW forces and separated by Na ions, as shown in Figure 1. Measurements of electrical resistivity and specific heat indicate the bulk nature of superconductivity with transition temperature (T_c) of 1.3 K for $NaSn_2As_2$ and 2.0 K for $Na_{1-x}Sn_2P_2$. Temperature-dependent magnetic penetration depth [3] and thermal conductivity [4] of $NaSn_2As_2$ indicate that the superconducting state can be classified into a fully gapped *s*-wave state with atomic-scale disorder.
In 2018, Cheng et al. reported the T_c of $NaSn_2As_2$ as 1.6 K [4], which is slightly higher than that reported in our previous work. Furthermore, they observed charge-density-wave-like anomaly in resistivity and specific heat at around 190 K. We found that off-stoichiometry in this compound, namely, Na doping on the Sn sites ($Na_{1+x}Sn_{2-x}As_2$) increases T_c to around 2.1 K [5]. Local structure analysis using extended X-ray absorption fine structure also detected the anomaly at around 190 K [6]. In the conference, we discuss detailed electronic structure of SnPn-based layered materials, as well as the synthesis of novel compounds.



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Keywords: pnictide, layered structure

PC2-2

Superconductivity with strong electron-phonon coupling in noncentrosymmetric W_3Al_2C

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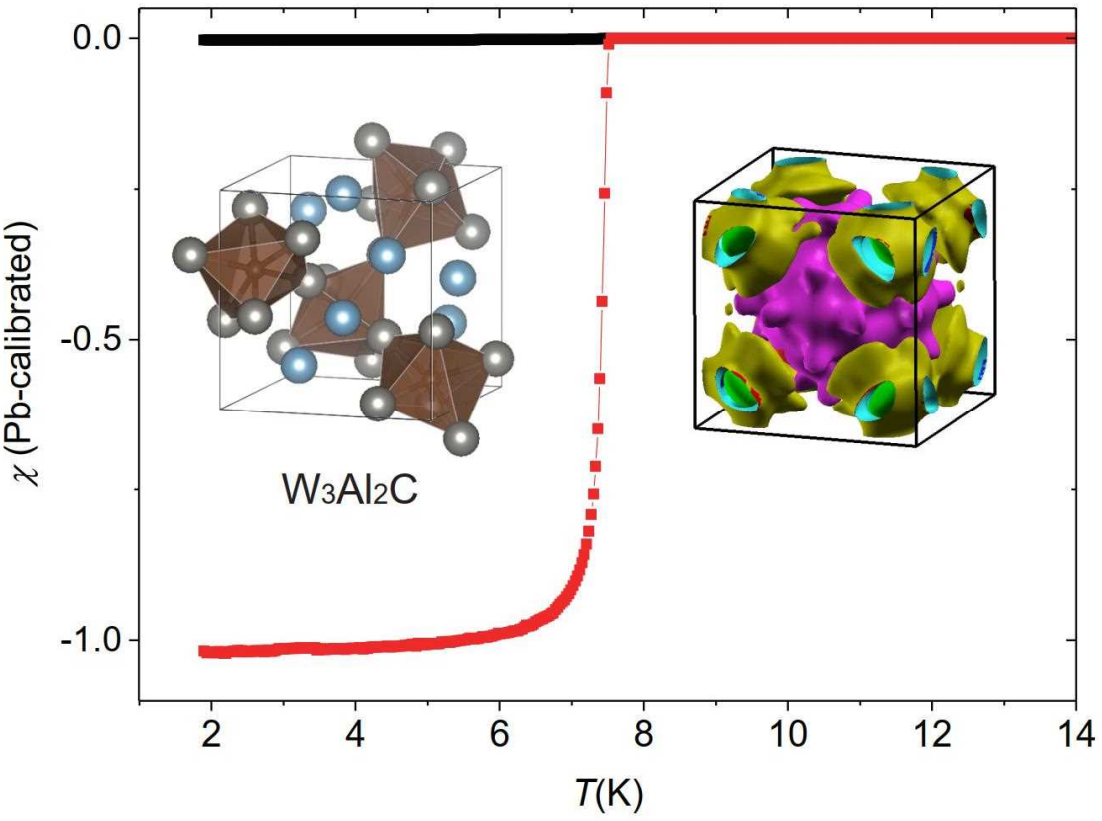
We report the discovery of superconductivity in W_3Al_2C (T_c = 7.6 K) synthesized by high-pressure method. W_3Al_2C is isostructural to Mo_3Al_2C (space group $P4_132$) but with stronger spin-orbit coupling (SOC). Different from the Mo_3Al_2C with metallic nature, the resistivity of the normal state of W_3Al_2C shows a non-metallic behavior. A specific heat jump of $\Delta C_{es}/\gamma T_c = 2.7$ and gap energy of $2\Delta(0)/\gamma T_c = 5.43$ are observed, which are much larger than that of Mo_3Al_2C (2.1 and 4.03) and the expectation of the Bardeen-Cooper-Schrieffer (BCS) theory (1.43 and 3.52). However, the Sommerfeld coefficient of W_3Al_2C is less than half of that of its Mo counterpart and the specific heat below T_c shows a power-law divergence following $C_{es}/\gamma T_c \sim (T/T_c)^{3.3}$ rather than an exponential relation. Theoretical calculations show that the Fermi surface of W_3Al_2C is dominated by W-5*d* electrons and the inclusion of SOC significantly changes its band structure, density of states (DOS) and Fermi surface topology. The realization of superconductivity by replacing 4*d* Mo towards 5*d* W provides a candidate for the search of potential triplet superconductors with enhanced SOC.



Keywords: superconductivity, noncentrosymmetric, spin-orbit coupling

PC2-3

Pressure-induced superconductivity and topological quantum phase transitions in topological materials

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Superconductivity and topological quantum states are two frontier fields of research in modern condensed matter physics. The realization of superconductivity in topological materials is highly desired; however, superconductivity in such materials is far from being thoroughly investigated. In this talk, we will discuss the electronic properties of some topological materials by applying high pressure. Pressure-induced topological quantum phase transitions and superconductivity is observed in some topological materials. The superconducting transition temperature Tc increases with applied pressure and a dome like phase diagrams were observed, which provides insights into the interplay between superconductivity and topological physics. Our theoretical calculations suggest the presence of pressure-induced topological quantum phase transitions as well as a structural–electronic instability.

Keywords: Superconductivity, High pressure, Topological materials

PC2-4

Effective model construction of $LaNiO_2$; a possible nickelate analogue of the cuprate superconductors

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Searching for analogues of cuprates has been considered as a possible path toward discovery of new high-T_c superconductors. An infinite layered nickelate $LaNiO_2$ has been considered as a possible candidate for such an analogue of cuprates because of its d^9 electron configuration [1,2]. First principles calculations have shown that the $d_{x^2-y^2}$ bandwidth is narrower than that of the cuprates, and in addition, two electron pockets originating from La 5d orbitals are present. In the present study, in order to study the possibility of superconductivity in $LaNiO_2$, we construct an effective two-orbital model for $LaNiO_2$ that takes into account the Ni $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ orbitals. Such a model has been constructed for the cuprates by some of the present authors, which lead to a successful reproduction of the experimentally observed trend of T_c [3]. The on-site interactions are estimated within the random phase approximation [4,5]. The estimation of the interaction parameters for the nickelate shows that the on-site interaction within the $d_{3z^2-r^2}$ orbital is relatively small due to its hybridization with the La orbitals. The fluctuation exchange study for the two-orbital model of $LaNiO_2$ results in d-wave superconductivity similarly to the cuprates, with a somewhat reduced T_c due to the narrower bandwidth.

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Keywords: Superconductivity, Cuprates, First-principle calculation, Hubbard model