Investigation of charge-density wave (CDW) in phosphate tungsten bronzes

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Abstract

In the last few decades physics of quasi-low-dimensional systems have triggered enormous interest among the physicists and the main reason for such studies is that low dimensional systems have a strong structural anisotropy, which is well reflected in their transport properties that exhibit uncommon features such as anomalous magnetic properties, metal-insulator and metal-metal transition, periodic lattice distortions, and charge-density-wave (CDW) phase transitions. Mono-phosphate tungsten bronzes ($MPTB_p$) are one such family of metallic bronzes with quasi-low-dimensional structural and electronic properties. The $MPTB_p$ family has the general formula $(PO_2)_4(WO_3)_{2m}$, where *m* is an integer (2, 4-16). The electronic structure of this family is interesting since the electronic and the magnetic properties of the members of this family strongly vary with *m*. We have chosen $P_4W_{12}O_{44}$ (*i.e* $m = 6$) for our studies which has an orthorhombic crystal structure. It consists of infinite ReO_3-type slabs of corner sharing WO_6 octahedra connected by PO_4 tetrahedra forming layers in the *ab* plane and are thus referred as quasi-two-dimensional systems. The structure leads to anisotropic physical properties as reflected in their electrical resistivity as well as the magnetic susceptibility measurements, which show two anomalies at T_{c1}=120 K and T_{c2}=60 K temperatures. It has been found that the anomalies in the transport properties of quasi-low-dimensional systems are always explained by CDW transitions and the CDW states are driven by nesting topology of the Fermi surface. Therefore, it is expected that the observed anomalies in $P_4W_{12}O_{44}$ (*i.e* $m = 6$) arise from the CDW instabilities. Hence, a detailed study on the electronic structure of these bronze systems can establish the origin of these observed anomalies in the transport properties.

We have performed high-resolution angle-resolved photoemission spectroscopy (ARPES) and density functional *ab-initio* theoretical calculation to study the electronic structure of $P_4W_{12}O_{44}$. We have experimentally determined the band dispersions and Fermi surface topology of $P_4W_{12}O_{44}$ and compared with our theoretical calculations and a fair agreement has been seen between them. Our experimental as well as theoretical investigation has resolved the origin of transport anomalies in these bronzes. The Fermi surfaces of these bronzes consists of flat patches, which can be connected with each other by a constant nesting wave vector, *q*. The scattering wave vectors found from diffraction measurements match with these nesting vectors and the anomalies in the transport properties of these bronzes can be well explained by the evolution of charge density wave with a partial nesting between the flat segments of the Fermi surfaces.