DOCTORAL THESIS SUMMARY

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Ab-initio study of electronic structure of HTc-superconductors based on FeAs–compounds

This thesis presents results of the extensive first-principles calculations on electronic properties of several FeAs-based superconductors. This work has particularly emphasized on the magnetic stability and the mechanism leading to the high-Tc superconductivity in $SrAFe_4As_4$ (A = Rb, Cs), $CaAFe_4As_4$ (K, Rb, Cs), and $Sr_4V_2O_6Fe_2As_2$ materials. Moreover, investigations of the optical and phonon properties of $SrRbFe_4As_4$ have also been conducted. All calculations were performed applying the Full Potential Linearized Augmented Plane wave (FP-LAPW) method implemented in ELK code, and also by the Projector-Augmented Wave (PAW) method employed in VASP package. The obtained data discloses some significant features of the systems studied.

Firstly, the DFT calculations within the PBE-GGA approximation and the spin-orbit coupling have been carried out for (Sr, Ca)AFe_4As_4 for the first time. The obtained data suggest the non-magnetic ground-state in these materials. Based on the density of states (DOS), it was found that the Fe-*3d* orbitals mainly contribute to the high DOS values around the Fermi level (E_F) and form the Van Hove singularity. This finding suggests an electronic instability, which actuates the superconductivity. The electronic band structure result shows numerous bands crossing the Fermi level and forming both hole- and electron-type pockets of the Fermi surface. A larger number of crossing E_F bands in 1144, compared to those in the parents $SrFe_2As_2$, $CaFe_2As_2$, AFe_2As_2, indicates a stronger inter-band scattering that is a necessary adjunct for the T_C enlargement in these superconductors. Concomitantly, their Fermi surfaces exhibit the shape of $^{\pm}s$-wave gap type contributed by several hole-type cylinders around the center Γ and electron-type sheets at the corner of the Brillouin zone. Particularly, the hole-type sheets of $SrRbFe_4As_4$ and $CaCsFe_4As_4$ are very much reminiscent of those in an unconventional nodal *d*-wave gap superconductor with the tiny width at some places. Besides, the ELF map expresses the high anisotropic distribution of electrons in 1144 compounds with the presence of both metallic bonds between Fe atoms and covalent bond of As-As, A-As. Furthermore, the ELF value in 1144 is lower than those in 122 indicating the weaker covalent bond. In other words, the broken covalency could be associated with the high-T_C superconductivity formation.

Secondly, the magnetic stability and electronic properties of $Sr_4V_2O_6Fe_2As_2$ were performed through the PBE-GGA approximation and LDA + U method.

• A comparison of electronic structure properties between two different incommensurate anti-ferromagnetic configurations (i-AF1, i-AF2) and the non-magnetic phases of $Sr_4V_2O_6Fe_2As_2$ was done applying FP-LAPW method. The self-consistent calculation predicts that i-AF2, having the lowest total energy, could be the most stable state in $Sr_4V_2O_6Fe_2As_2$ among these considered phases. The density of states divulges the more unstable electrons in the nonmagnetic phase than those in others with the complicated peak structure just below the Fermi level. Especially, the partial densities of states shows no magnetic arrangement of Fe atoms but strong AF ordering of V atoms with the moment of 1.25 μB/1 V at. Generally, the density of states around the Fermi level is dominated by Fe and V atomic contributions. Therefore, that is not only Fe electrons, like in 1144 materials, but also V electrons participate in the superconducting state creation in this compound. The higher number of electronic bands crossing E_F in i-AF than those in NM state suggests stronger inter-band scattering in magnetic phases. These features actually point out the coexistence of magnetism and superconductivity in $Sr_4V_2O_6Fe_2As_2$. Remarkably, the Dirac-cone-like structure with a small gap was found between the bands in the vicinity to E_F. The Fermi surfaces of $Sr_4V_2O_6Fe_2As_2$ show the multi-sheet character containing the hole-type sheets at the center and electron-type ones in the corner of the Brillouin zone. However, Fermi surfaces topologies are completely different from one to another following the change of the magnetic vector. The Fermi velocities map manifests the highly anisotropic distribution of electrons that contribute to both horizontal and vertical nodal lines in this superconductor.

• The stability of A-type (A-AF) and checkerboard (c-AF) anti-ferromagnetic configurations $Sr_4V_2O_6Fe_2As_2$ upon the influence of on-site $d-d$ Coulomb interaction U and magnetic correlation J was studied using the supercell approach within the LDA + U method. It was found that the magnetic stability of these phases strongly depends on the value of (U, J). Similar to the previous study on the i-AF phases, the Fe atoms in $Sr_4V_2O_6Fe_2As_2$ exist in the non-magnetic state. Whereas, the magnetic arrangement occurs only in the network of V sites with the magnetic moment value around 1.3 μB/1 V at. in the A-AF and 1 μB/V in the c-AF structures. Similarly to the case of 1144 superconductors, the ELF picture of $Sr_4V_2O_6Fe_2As_2$ exhibits the highly anisotropic behavior of electrons distributions amongst the separate atoms involved in the compound. That shows a more localized character of electrons around As, Sr, O than that itinerant one coming from V and Fe atoms. The DFT data allow the conclusion that Fe-*3d* and V-*3d* electrons mostly take part in the Cooper pairing in $Sr_4V_2O_6Fe_2As_2$.

Finally, the optical and phonon properties of $SrRbFe_4As_4$ were examined through the PAW method with the PBEsol-GGA exchange-correlation functionals. Very first time

that we have calculated dielectric function, refractive index, extinction coefficient, absorption, energy-loss, reflectivity and optical conductivity. Based on the data we have determined some important parameters of the optical and phonon properties, such as electron-phonon coupling, plasma frequency and effective number of carriers participating in the optical transitions. On the whole, the optical parameters display the highly anisotropic behavior and strong response under the infrared and visible lights, which originates from the intra-band and inter-band transition of Fe-*3d* and As-*4p*. It is expected to observe the transparent state of $SrRbFe_4As_4$ when the incident irradiation energy higher than 63 eV, where the imaginary dielectric function falls down to zero. Otherwise, low reflectivity and a high absorption coefficient imply the good absorption of this material. Whereas, the phonon dispersion with no imaginary part conveys the dynamical stability and the phonon density of states discloses the strong vibration of Fe and As atoms. Furthermore, a large electron-phonon coupling and the phonon anomaly indicate the strong coupling in this superconductor. Thus, the optical and phonon properties in $SrRbFe_4As_4$ are significantly affected by FeAs-layers that support their crucial role in the high-T_C superconductivity of this material. In our opinion, the obtained data could expand our knowledge of the superconductivity in the high-T_C $SrRbFe_4As_4$ material. However, the related experiments are strongly required in order to verify our theoretical data. Obviously, systematic study aiming to evaluate, and summarize the findings of all relevant superconductors is highly desired in the further investigations. Also DFT investigations of physical properties of other materials are highly desired.