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授与した学位	博　士
専攻分野の名称	理　学
学位授与番号	博甲第　　６８３５　　号
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学位授与の要件	自然科学研究科　　学際基礎科学専攻 （学位規則第４条第１項該当）
学位論文の題目	Theory for superconductivity and magnetism in layered titanium and chromium based materials （チタン系およびクロム系層状化合物における超伝導と磁性の理論）
論文審査委員	教授　市岡　優典　　教授　久保園　芳博　　准教授　小林　夏野

学位論文内容の要旨

In chapter 1, we introduce the background of superconductor and superconductivity, previous studies and crystal structure of titanium-based superconductors and ternary chromium tellurides.

In chapter 2, one of the most powerful theories for today's studies of many-body system, the density functional theory (DFT) is introduced. We give the details of Kohn-Sham auxiliary system and Generalized-gradient approximations (GGA). Moreover, basis of Full-potential local-orbital (FPLO) minimum-basis is discussed.

In chapter 3, beyond DFT, we introduce the random phase approximation to realize the spin fluctuation theory, in which the electron-electron interaction is considered. In this framework, we exhibit the derivation of susceptibilities and two-electron pairing vertex.

In chapter 4, we discuss another method for strongly correlated systems, the dynamical mean-field theory, which is a useful method to calculate finite temperature cases and to compare with experimental results.

In chapter 5, results of titanium oxypnictides are exhibited. We mainly study the $Ba_{1-x}A_xTi_2Sb_2O$ with varying alkali-doping (A=Na, K, Rb). Using density functional theory, we determine density of states and band structure with the orbital character. However only using the density of states at the Fermi-level $N(E_F)$ cannot explain the evolution of the superconducting T_c, which indicates that transition temperatures may not be accounted for by an electron-phonon mechanism. Then we extract a tight-binding model for $Ba_{1-x}A_xTi_2Sb_2O$ by using projective Wannier functions and apply the random phase approximation to calculate susceptibilities and pairing vertex for revealing the superconduct-ing order parameters of the gap function, which successfully explains the tendency of T_c by leading eigenvalue λ and gives the symmetry of superconducting order parameters that shows sign-changing s-wave unconventional supercon-ductor.

In chapter 6, we study the insulator-metal transition of $CrGeTe_3$ along increasing pressure. By using DFT with GGA+U, we obtain the evolution of Curie-Weiss temperature θ_{cw} that is comparable with experiment result. Then by using DFT+DMFT we show the insulator-metal transition on spectral function at finite temperature, which is a good result to compare with angle-resolved photoemission spectroscopy (ARPES) results from experiment.

In chapter 7, we make a summary of this thesis and discuss prospects for future work.

論文審査結果の要旨

In this Thesis, the candidate reports his theoretical research about (1) the alkali doping dependence of electronic states and superconductivity in titanium-based layered compounds $Ba_{1-x}A_xTi_2Sb_2O$ (A=Na, K, Rb), and (2) pressure dependence of the magnetism and metal-insulator transition in a chromium-based layered compound $CrGeTe_3$. These materials belong to 3d electron system like cuprates and iron-based superconductors. The theoretical studies are performed by several methods, including density functional theory (DFT), spin-fluctuation theory, and dynamical mean-field theory (DMFT).

In the study on $Ba_{1-x}A_xTi_2Sb_2O$ with varying alkali-doping x (A=Na, K, Rb), he calculates electronic states by DFT, and reveals contributions of 3d and 5p orbitals in the band structure and the Fermi surface. For estimate of the superconducting transition temperature T_c by the spin fluctuation theory, 26-orbital tight-binding model is constructed from the DFT results, and the magnetic susceptibility and the leading eigenvalue of the gap equation are calculated. Since the results reproduce tendency about the doping-dependence of T_c, it is suggested that the superconducting pairing mechanism may come from spin fluctuations, and that the possible pairing symmetry is the sign-changing s-wave.

In the research on $CrGeTe_3$, the electronic state is calculated by DFT, and the pressure dependence of the Curie-Weiss temperature is obtained by evaluating the exchange coupling coefficient of the Heisenberg model. Using DMFT, he also discusses the pressure dependence of metal-insulator transition and the spectral function which can be compared with experimental ARPES results.

The committee evaluated the quality of the research by the document of Dissertation and the presentation in the Thesis defense. In the defense, the presentation was nicely done in English, and questions to the presentation were reasonably answered. The research outcomes by the candidate give valuable contributions in the research field of superconductivity and magnetism in layered titanium- and chromium-based materials. Therefore, the committee concludes that the candidate passes the Thesis defense for Doctor of Philosophy in Science.