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Theoretical study of novel superconductivity in Ir oxides with large spin-orbit coupling HIROSHI WATANABE, TOMONORI SHIRAKAWA, SELJI YUNOKI, RIKEN, CREST, COMPUTATIONAL CONDENSED MATTER PHYSICS LABORATORY, RIKEN ASI TEAM, CREST, JAPAN SCIENCE AND TECHNOLOGY AGENCY TEAM, COMPUTATIONAL MATERIALS SCIENCE RESEARCH TEAM, RIKEN AICS TEAM — Recently, the $5d$ transition metal oxide Sr_2IrO_4 has attracted much attention. In this material, three t_{2g} orbitals of Ir atoms are hybridized with each other by the spin-orbit coupling of $5d$ electrons. As a result of the quantum entanglement of spin and orbital degrees of freedom, an anomalous $J_{\text{eff}}=|L-S|=1/2$ state is realized, which causes interesting properties. To clarify the properties of this system, we have studied the ground state of the three-orbital Hubbard model with a spin-orbit coupling term using variational Monte Carlo method. Here, we study the electronic states when carriers are doped in this three-orbital system and discuss the possibility of superconductivity. The obtained ground state phase diagram reveals the antiferromagnetic state, stable around the electron density $n=5$, is destabilized by carrier doping and the ground state turns to be superconducting under a certain condition. Similar to the high- T_c cuprates, a large asymmetry between electron doping ($n > 5$) and hole doping ($n < 5$) is also observed. Due to the large spin-orbit coupling, the spin is no longer a good quantum number. Instead, the pseudospins form a Cooper pair and a $d_{x^2-y^2}$ -wave “pseudospin-singlet” superconductivity is realized.

Hiroshi Watanabe
RIKEN, CREST

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