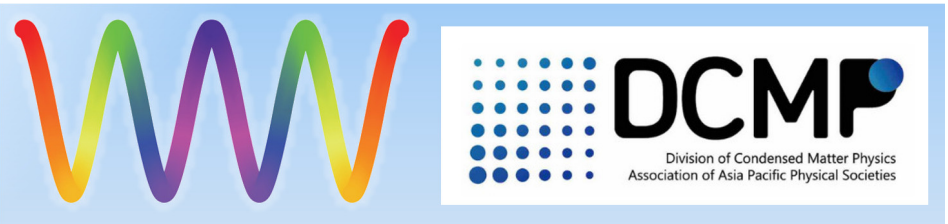

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Electronic structures and superconductivity of new RP-type nickelate superconductors

The recently discovered Ruddlesden-Popper bilayer superconductor La3Ni2O7 has attracted widespread attention due to its high Tc˜80 K under a pressure. Soon after that, the trilayer La4Ni3O10 was found to show superconductivity at high pressure too. Our density functional theory calculations indicate that the 3dx2−y2 and 3dz2 orbitals of Ni cations mixing with oxygen 2p orbitals play critical role in the emergence of superconductivity in the bilayer and trilayer nickelate superconductors, especially the apical oxygen ions forming the Ni–O–Ni bonds. We propose a bilayer two-orbital model for La3Ni2O7 under high pressure, primarily based on the 3dx2−y2 and 3dz2 orbitals of Ni. Through Wannier downfolding and symmetry analysis, we obtain parameters such as electron hopping and site-energy, which provide an excellent description of the electronic band structure and Fermi surface. To explicitly consider the physics of O-p orbitals, we further introduce a higher energy model (11-orbital model). Based on these models, we study the charge transfer, Zhang-Rice singlet bands, pairing symmetry, and superconducting transition temperature in La3Ni2O7. We obtain a comprehensive superconducting phase diagram in the doping plane and find that the La3Ni2O7 under pressure is situated roughly in the optimal doping regime of the phase diagram. We perform a first-principles study of La4Ni3O10 for both the P21/a phase at ambient pressure and I4/mmm phase at high pressure. Our results show the characteristic upward shift of a Ni-3dz2 bonding band under pressure in La4Ni3O10. We propose a trilayer two-orbital model by performing Wannier downfolding on Ni-eg orbitals. According to the model, our calculated spin susceptibility under RPA shows that the 3dx2−y2 orbital is also important for the magnetic fluctuation in the RP series. Moreover, a high energy 16-orbital model with direct dp, pp hoppings is proposed, which implies that La4Ni3O10 also lies in the charge-transfer picture. Our exposition of electronic reconstructions, multiorbital models and superconductivity shed light on theoretical electronic correlation study and experimental exploration of superconductors in the RP series.

Field of Condensed Matter

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