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Electron Correlation Effects And The Electronic Structures of Perovskite Ruthenates SrTi1-xRuxO3 PAO-AN LIN, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan, T.Y. CHANG, Department of Physics, National Tsing Hua university, Hsinchu, Taiwan, HORNG-TAY JENG, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan and Department of Physics, National Tsing Hua university, Hsinchu, Taiwan, CHEN-SHIUNG HSUE, Department of Physics, National Tsing Hua university, Hsinchu, Taiwan — The behavior of the electronic structures of SrTi1-xRuxO3 crystals as the value of x is varied, were studied by ab initio LDA band structure calculation. The roles of on-site Coulomb interaction U were included by carrying out LDA+U calculations. It is found that electron correlation effects play an important role in the electronic structures involving the Ru4d orbitals in the Perovskite ternary Ruthenates SrTi1-xRuxO3. The on-site Coulomb interaction U is needed to describe correctly the metal- insulator transition. Comparing with LSDA calculation (including GGA(generalized gradient correction),the calculated spectrum from LDA+U band structure calculation are in much better agreement with published experimental results such as photoemission (PES) and oxygen 1s X-ray absorption (XAS) spectroscopy for clean surface.

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