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Oxygen divacancy in perovskite oxides

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The first principles calculation is used to study oxygen divacancy in titanate materials $ATiO_3$ (where A is Sr, Ba and Pb). In this study, the LDA+U is applied to address the strongly correlated effects of defective electrons. The values of Coulomb interaction (U) and exchange interaction (J) from U −J = 0 eV (LDA) to U −J = 4.36 eV were used. We found that the lattice parameter and band gap are expanded with increasing the U-J parameters. When two oxygen vacancies are removed from the lattice, the defective band shift down under Fermi level leading to the formation of the localized state in band gap at specific configuration on both three materials. This study also suggests that the oxygen vacancies clustering may lead to the further localization of defective electrons.

Keywords: Perovskite, Oxygen vacancies, electronic structure, LDA+U

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Mass Production of Metal Nanoparticles for the Application of Electronic Device

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The synthesis and characterization of metal nanoparticles have attracted a great deal of attention due to their potential application in electronics, optics, and catalyst. However, the synthesis of high concentrated and large scaled metal nanoparticles was difficult from the absence of the effective starting material as a precursor and reducing agents as a reductant. The development of synthetic pathway to produce a highly yield nanoparticles is an important aspect of industrial technology. Herein, we report a simple, rapid approach to synthesize organic-soluble Cu and Ag nanoparticles in colloidal method for the application in a conductive pattern using inkjet printing. The silver nanoparticles have been synthesized in highly concentrated organic phase because copper (II) acetylacetonate (Cu(acac)2) is effective reducing reagent for the creation of homogeneous nucleation process. The Cu nanoparticles have been synthesized by the reducing of the copper oxide materials using acid molecules in high concentrated organic phase. We have made high concentrated metal nanoinks which contain the metal nanoparticles above ~50 wt% due to their highly stable dispersibility. Furthermore, their sintering and electric conductivity properties were investigated by melting process between 200°C and 250°C for application to printed electronics.

Keywords: nano, silver, copper, nanoink