Ab-initio calculations of pressure effect on electronic and magnetic structure of ferromagnetic-superconductor RuSr$_2$GdCu$_2$O$_8$

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Abstract
We have performed a first-principle calculation of electronic structure of RuSr$_2$GdCu$_2$O$_8$, a ferromagnetic-superconductor, by employing a full-potential linearized augmented plane-wave method within the density functional theory. Hydrostatic pressure applied up to 6 GPa by varying the volume of the unit cell with constant a:b:c ratio. Optimization of internal parameters showed that there exists shear stress due to the residual forces in Ru-O layers which leads to anti-phase rotation of RuO$_6$ octahedra in experimental structure of this compound. Partial charge analysis showed that applying pressure leads to hole injection in Cu-O sheets and by applying charge transfer model, we obtained 1.9 K/GPa for the rate of increase in superconducting transition temperature with pressure. The exchange coupling interaction J between the adjacent Ru atoms was calculated by energy difference between the AFM and FM configuration of magnetic structure of Ru atoms. According to the result of the calculations, the magnetic moment of Ru atoms decreased and exchange coupling parameter J increased by applying pressure.

Keywords: carbon nanotubes, CNTs, arc discharge, Raman spectroscopy

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