DFT-based derivation of the microscopic model for the frustrated antiferromagnet Cs_2CuCl_4

K. Foyevtsova, Y. Zhang, H. Jeschke and R. Valentí

Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue Str. 1, 60438 Frankfurt am Main, Germany, E–mail: foyevtsova@itp.uni-frankfurt.de

Recent experiments on the layered $S = 1/2$ frustrated antiferromagnetic compound Cs_2CuCl_4 indicate that in this material an exotic spin liquid (SL) state with fractional-spin quasiparticles might be realized. Even more fascinating is the fact that the analysis of the magnon dispersion spectrum in this system leads to the conclusion that Cs_2CuCl_4 can be described by a 2D triangular lattice of magnetic interactions. Whether the above mentioned SL state can exist in two dimensions is still a matter of debate among theoreticians. It is therefore clear that in order to develop a solid connection between theory and experiment an alternative determination of the microscopic model, such as by, e.g., the Density Functional Theory (DFT) method, for Cs_2CuCl_4 would be of great value.

In this presentation, we discuss the microscopic model for Cs_2CuCl_4 derived with the DFT approach. We also perform downfolding and tight-binding calculations and discuss the role of the electronic correlations in the compound. We find that inclusion of the on-site Coulomb interaction U for the Cu $3d$ electrons during the crystal structure relaxation is important in order to have agreement with the experimental observations.