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Electronic structure of the quasi-two-dimensional spin-gap system $SrCu_2(BO_3)_2$ ANDRES SAUL, CINaM/CNRS (Marseille, France), GUILLAUME RADTKE, IM2NP (Marseille, France), H. DABKOWSKA, B. GAULIN, G. BOTTON, McMaster University (Ontario, Canada) — During the last decade, a lot of theoretical and experimental work has been devoted to the study of the magnetic properties of $SrCu_2(BO_3)_2$. This compound crystallizes in a tetragonal structure where layers of $CuBO_3$ alternate with planes of Sr atoms along the(001) direction. Due to this unusual structure where Cu^{2+} atoms are arranged in the layers to form a network of orthogonal dimers, $SrCu_2(BO_3)_2$ appears as the first realization of a 2D Heisenberg model known as the Shastry-Sutherland model and exhibits a number of unique features such as a spin gap behavior, unusual magnetic excitations or a magnetization *plateaux*. In this work, the electronic structure of this system has been investigated using first-principles band structure calculations within the local-density approximation (LDA)+U method as implemented in the `wien2k` code. The comparison of our calculations with available experimental data (exchange integrals estimated from magnetic susceptibility measurements, optical gap from reflectance measurements, and O-K edge recorded in EELS) shows that the (LDA)+U method with a single value of the parameter U can provide an accurate description of both low-energy-scale (magnetic) and high-energy-scale (electronic) properties of this magnetic insulator.

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