Electronic structure of the quasi-two-dimensional spin-gap system \( \text{SrCu}_2(\text{BO}_3)_2 \) ANDRES SAUL, CINAM/CNRS (Marseille, France), GUIL- LAUME 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 \( \text{SrCu}_2(\text{BO}_3)_2 \). This compound crystallizes in a tetragonal structure where layers of \( \text{CuBO}_3 \) alternate with planes of \( \text{Sr} \) atoms along the(001) direction. Due to this unusual structure where \( \text{Cu}^{2+} \) atoms are arranged in the layers to form a network of orthogonal dimers, \( \text{SrCu}_2(\text{BO}_3)_2 \) 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 \text{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.