Experimental and theoretical investigation of the electronic structure of $CuAlO_2$ delafossite under high pressure

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In spite of the large interest aroused by the p-type transparent conductor CuAlO2 since its discovery [1], the nature and value of its band-gap remains controversial [2]. In this communication we report on the evolution of the electronic structure of $CuAlO_2$ delafossite under pressure and determine the value and character of its band-gap on the basis of optical measurements and ab-initio electronic structure calculations. The absorption spectrum in the NIR-VIS-NUV range has been measured on single crystals up to 20 GPa for light polarization perpendicular and parallel to the symmetry axis. In the near-infrared and visible range the absorption spectrum consists of several absorption bands that are proposed to be related to internal transitions in Cu^{+2} ions near to Cu vacancies. Absorption in the ultraviolet corresponds to the fundamental transition that exhibits a quadratic dependence on the photon energy, corresponding to an indirect gap of 2.95 eV at ambient pressure, that increases under pressure at a rate of 15 meV/GPa. At higher energy we detect the onset of an intense allowed transition that moves with a pressure coefficient 1.8 meV/GPa and was previously identified as the fundamental transition from absorption measurements on thin films.

References:

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