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ABSTRACTS

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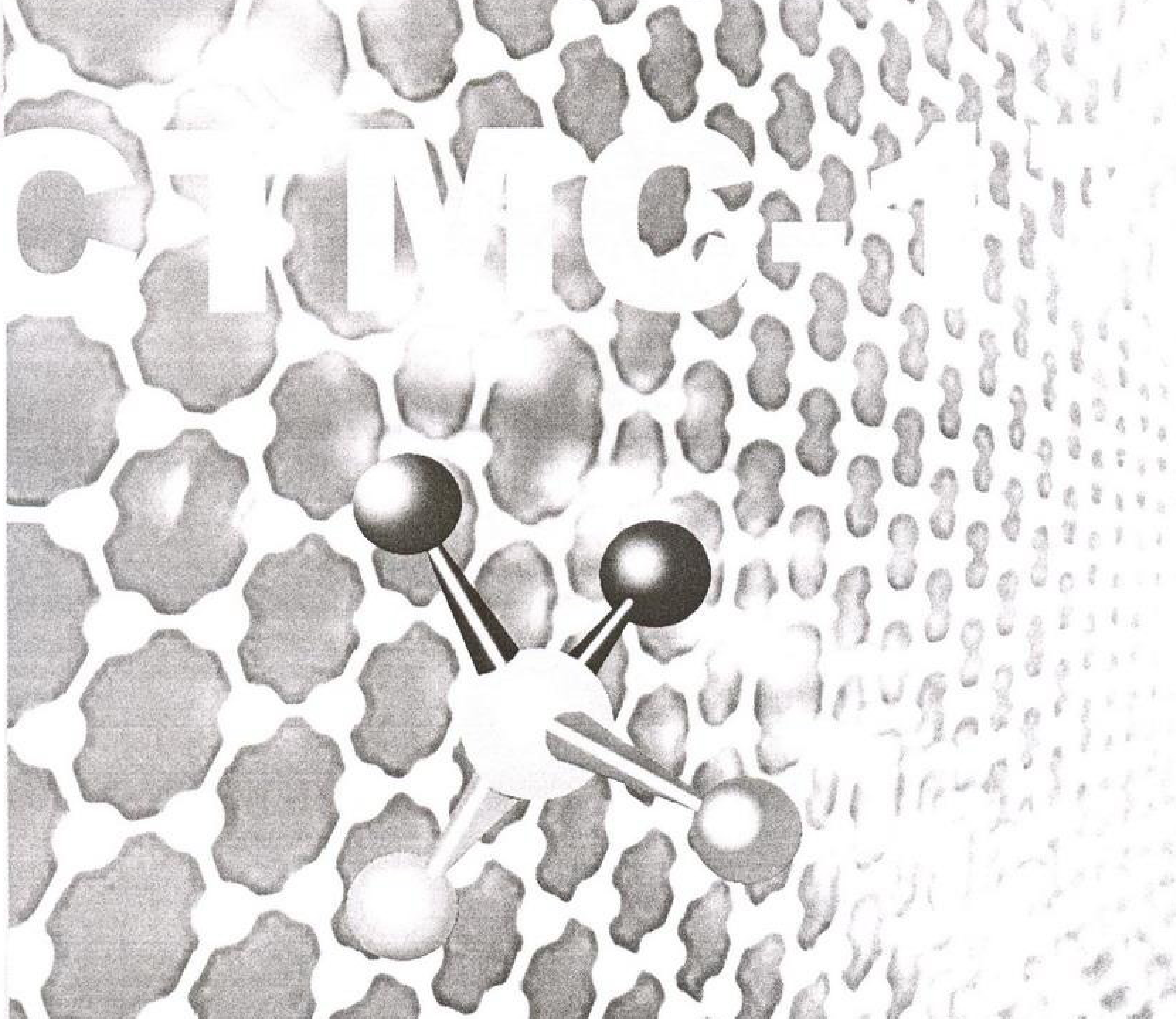

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Diamagnetic shift of the A free exciton in $CuGaSe_2$ in magnetic fields

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$CuGaSe_2$ is a promising chalcopyrite compound for the absorber layer of thin-film solar cells. In order to optimise the efficiency of $CuInSe_2$-based cells, $CuInSe_2$ is alloyed with $CuGaSe_2$, forming $Cu(In,Ga)Se_2$ (CIGS), to match the band-gap of the CIGS absorber layer to the solar spectrum. Current achieved efficiencies for CIGS-based solar cells saturate towards 20% [1] which is significantly lower than the theoretical limit for one-junction solar cells of 30%. To improve the device performance, it is essential to understand the fundamental physical properties of this material. The application of high magnetic fields can provide important information on the electronic properties of semiconductors. High magnetic fields have two effects on the excitonic energy levels. The first effect is the Zeeman spin-splitting and the second effect is a non-linear diamagnetic shift. The diamagnetic shift of an exciton can be used to estimate its binding energy, Bohr radius and reduced mass as well as the effective masses of the charge carriers. Single crystals of $CuGaSe_2$ were grown by the vertical Bridgman technique. Magneto-optical photoluminescence (MPL) measurements were carried out at the Grenoble High Magnetic Field Laboratory using a 20 T resistive magnet at 4.2 K. Fibre optics were used to transport the 514 nm line of an Ar^+ laser to the sample and the MPL to the entrance slit of a 0.5 m Princeton Instruments spectrometer and detected by a 1340 Silicon CCD.

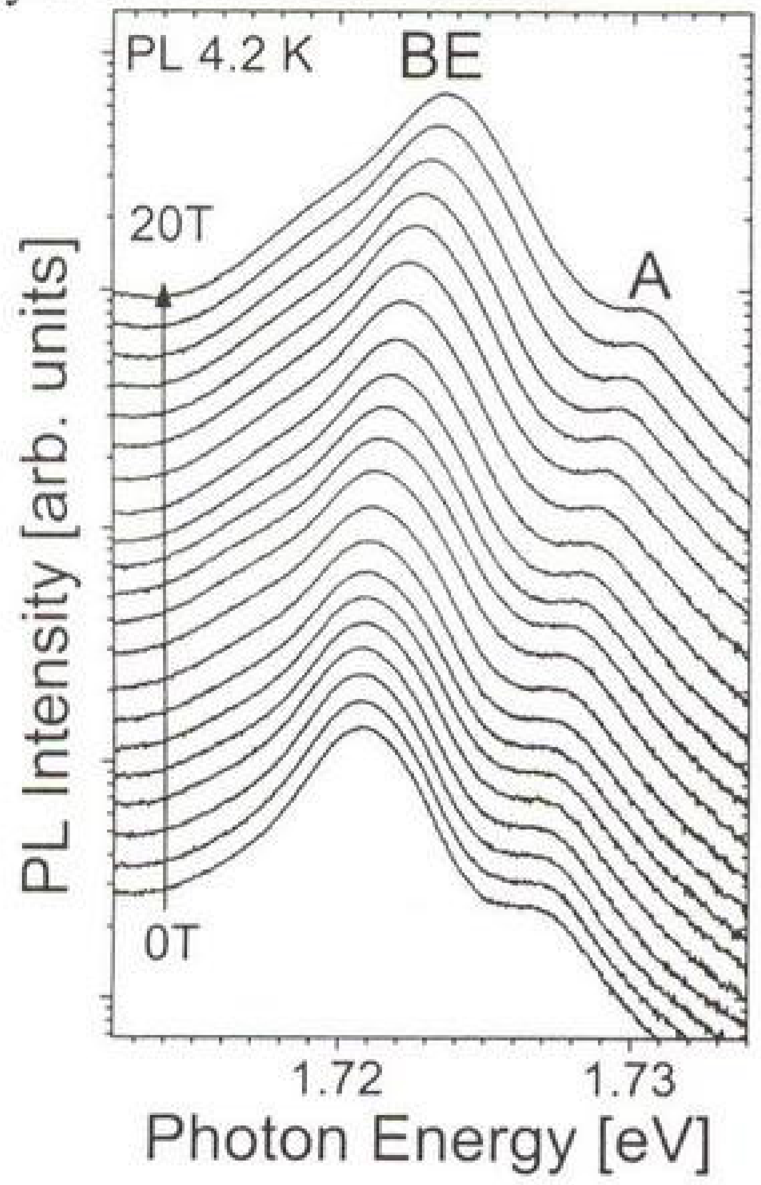

Fig. 1 Near band-gap PL spectra of $CuGaSe_2$ under magnetic fields from 0 to 20 T taken at 4.2K.

At zero magnetic field, the near band-gap PL of $CuGaSe_2$ taken at 4.2 K (Fig. 1) reveals two peaks A at 1.727 eV and BE at 1.721 eV which correspond to the A free exciton and to an exciton bound to a neutral acceptor [2], respectively. An increase in the magnetic field strength from 0 to 20 T results in a gradually increasing blue shift of both the bound exciton and the A free exciton, as shown in Fig. 1. Within the weak field approximation the magnetic field can be treated as a perturbation and the diamagnetic energy shift ΔE_d is given by [3]:

$$\Delta E_d = (e^2 a_B^2 / 4\mu) B^2 = (4\pi^2 \hbar^4 \varepsilon^2 \varepsilon_0^2 / e^2 \mu^3) \qquad (1)$$

From the evolution of the A free exciton PL peak position a diamagnetic shift rate c_d = 9.82 x 10^{-6} eV/T^2 has been determined. From equation 1 and with ε = 11 [2], a reduced mass μ = 0.115 m_0 of the A free exciton has been calculated which is less than the literature value μ = 0.125 [4, 5]. Assuming an effective electron mass of m_e = 0.14 m_0 [4] results in an effective hole mass of m_h = 0.64 m_0. An exciton binding energy of 12.9 meV and an exciton Bohr radius a_B = 5.07 nm have been calculated using the hydrogenic model.

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