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ABSTRACTS

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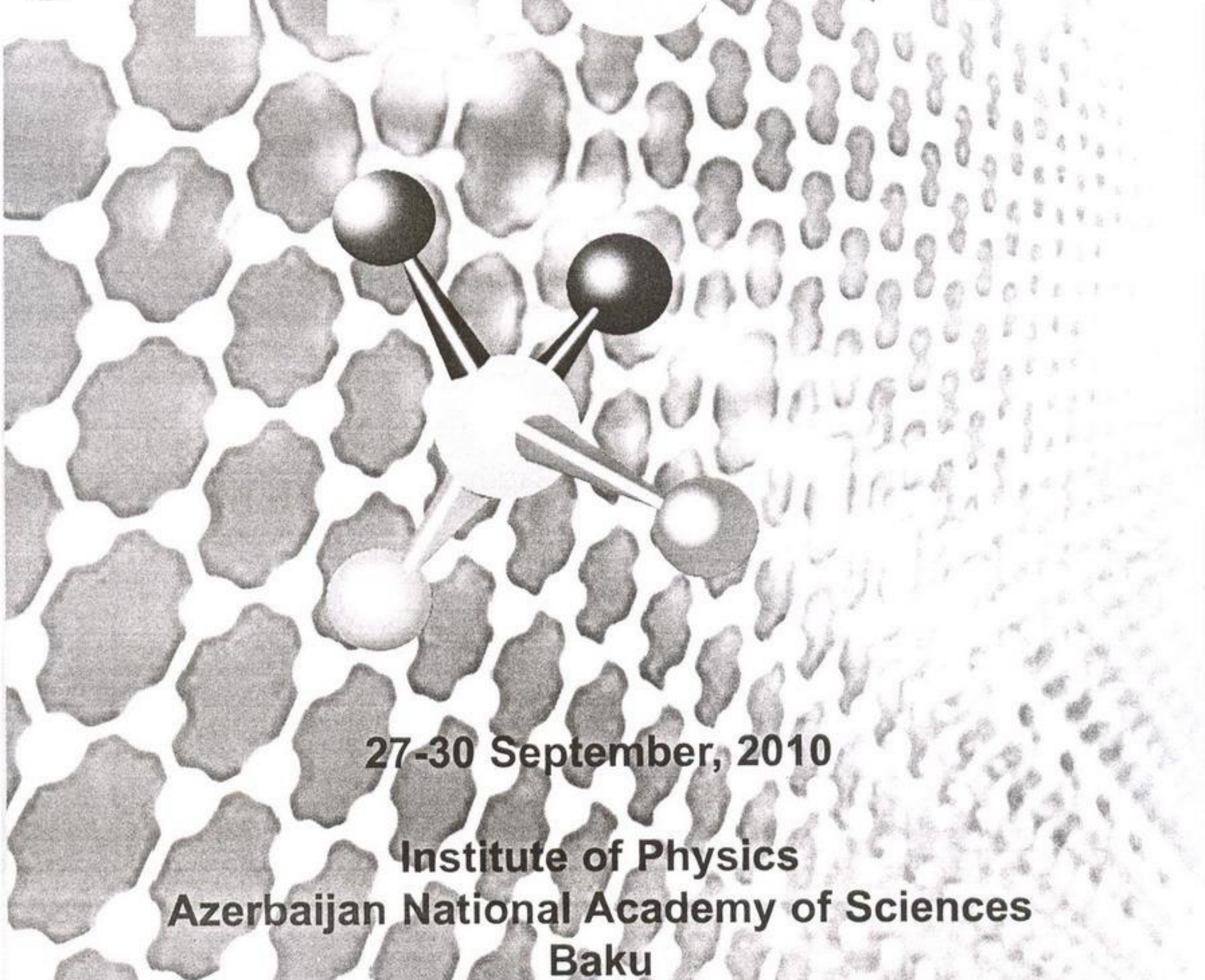

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Excited states of the A and B free excitons in $CuInSe_2$

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Solar cells with $CuInSe_2$-based semiconductor compounds in the absorber layer are amongst the leading thin-film technologies in terms of conversion efficiencies and stability. However, efficiencies for $CuInSe_2$-based solar cells currently saturate near 20% rather than 30%, which is the theoretical limit for a one-junction solar cell, suggesting a lack of fundamental understanding and control of these materials. One of the milestones in the development of every semiconductor material for optoelectronics applications is establishing properties of the free excitons and their excited states. It is difficult to underestimate the importance of such information since the spectral distance between the ground $E_{FE}(n = 1)$ and excited $E_{FE}(n = 2)$ states of the free exciton provides an accurate and independent value for the binding energy E_b of the exciton and thus for the band gap E_g, one of the most important parameters for any semiconductor, which is given by $E_g = E_{FE}(n = 1) + E_b$. Despite a significant amount of research on $CuInSe_2$ no information on the excited states of its free excitons can be found in the literature. Therefore the band gap in this material can not be considered as accurately established.

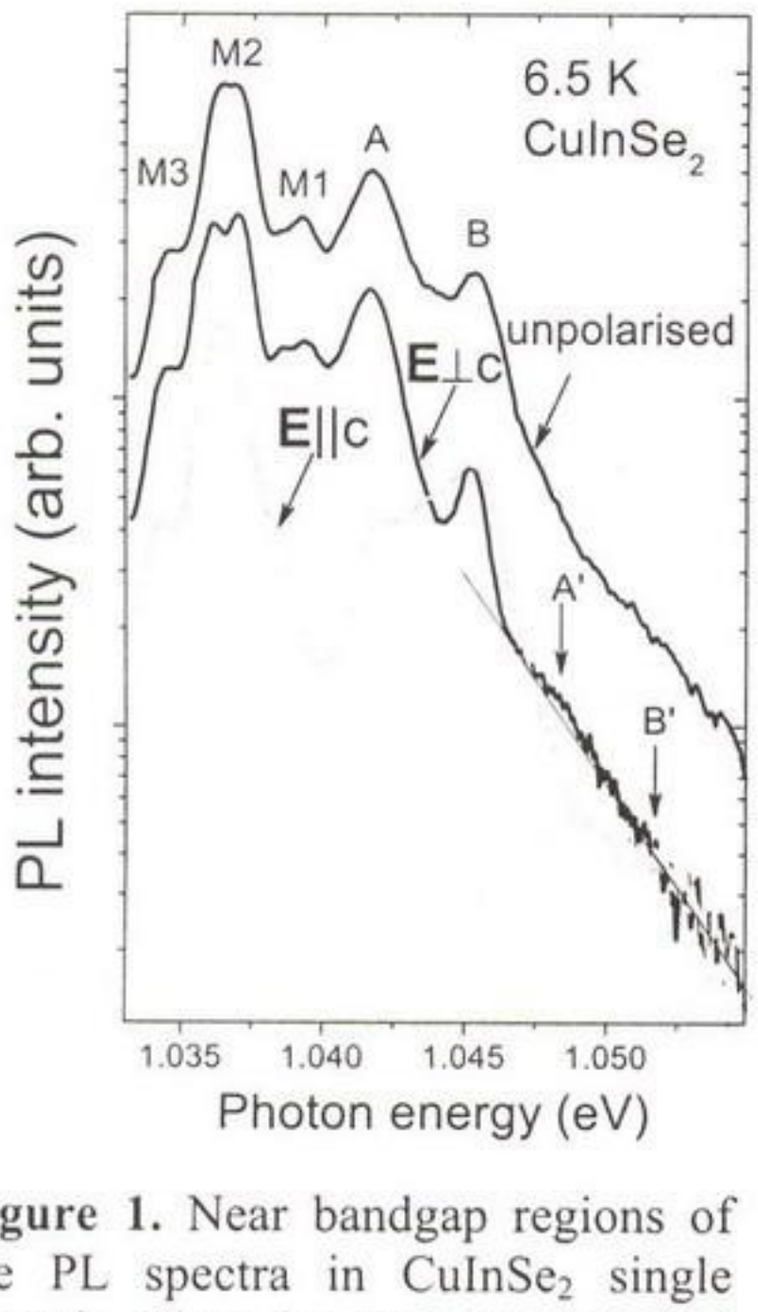

Figure 1. Near bandgap regions of the PL spectra in $CuInSe_2$ single crystals taken for the non-polarised as well as for $\mathbf{E}\perp c$ and $\mathbf{E}\parallel c$ polarised conditions. The A and B free excitons reveal their first (n = 2) excited states A' and B'.

Single crystals of $CuInSe_2$ were grown by the vertical Bridgman technique. Oriented samples were examined by polarisation resolved photoluminescence (PL) at 6.5 K. **Figure 1** shows the free exciton region of PL spectra with the polariser oriented perpendicular $\mathbf{E}\perp c$ and parallel $\mathbf{E}\parallel c$ to the c axis along with the unpolarised spectrum. The spectra reveal the A and B free excitons as well as the M1, M2 and M3 bound excitons as established earlier [1]. The A free exciton is polarised perpendicular to the c-axis, consistent with the $\Gamma_{6v} - \Gamma_{6c}$ transition selection rule [2]. The B exciton is represented by the $\Gamma_{7v} - \Gamma_{6c}$ transition, which is allowed in both the $\mathbf{E}\perp c$ and $\mathbf{E}\parallel c$ polarisations, and therefore its intensity does not change much as the polarisation changes. With the intensity of the A exciton minimised ($\mathbf{E}\parallel c$) the n = 2 excited state of B can be seen. With the intensity of the B exciton minimised ($\mathbf{E}\perp c$) the n = 2 excited state of the A exciton is resolved.

The energies of the first (n = 2) excited states for the A and B free excitons are 1.0481eV and 1.0516eV, respectively. Accurate values of the A and B exciton binding energies have been calculated assuming a hydrogenic model, giving $E_b^A = 8.5$ and $E_b^B = 8.4$ meV. The model also gives values for the Bohr radii $a_B^A = 7.5$, $a_B^B = 7.5$ nm as well as the static dielectric constant $\varepsilon = 11.3$. The bandgaps of the A and B excitons are estimated as 1.0502 eV and 1.0537 eV, respectively, at 6 K.

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