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Investigation into the electronic, optical and structural properties of Perovskites

Solar cells using inorganic/organic perovskites as the primary energy-harvesting materials have recently been shown to be very efficient, and have generated ongoing investigations into developing similar materials [1-3]. Two such materials that we have investigated are the perovskites Formamidinium Lead Iodide ($FAPbI_3$) and Caesium Lead Bromide ($CsPbBr_3$) through the use of Spectroscopy Ellipsometry (SE), X-ray Absorption Spectroscopy (XAS) and first-principle calculations. The electronic and optical properties of a band-gap tunable perovskite in the form of $FA_{0.85}Cs_{0.15}PbI_{2.9}Br_{0.1}$ show that it is more stable than the commonly used Methylammonium Lead Iodide ($MAPbI_3$), has a much lower exciton binding energy of (5.9 ± 2.0) meV, a strong electron-electron correlation and a much greater number of excitons and free carriers than most perovskites commonly used in solar cells, thus showing that $FA_{0.85}Cs_{0.15}PbI_{2.9}Br_{0.1}$ is a favourable alternative to $MAPbI_3$ [4,5]. Most importantly, we show that the large exciton density is due to the strong electron-electron interactions within the material. The perovskite $CsPbBr_3$ is a promising new nano-crystalline material that has been utilised in next-generation photo-voltaic cells, emission devices and even Gamma and X-ray detection units [6-8]. The optical and electronic properties of the nano-crystalline perovskite, including the exciton binding energy, average nano-crystal size, temperature coefficients, optical transitions and electron-electron correlations are revealed. It was found that the material exists in a dual structural phase from 361K down to 7K, which is an effect of the materials nano-crystalline nature. A sudden change in the electronic structure at 150K – 160K was found to occur because the rate at which the nano-crystals transition from the tetragonal to orthorhombic phase is non-linear with temperature. This has far-reaching implications for nano-crystalline materials in nano-technology and our novel method of calculating the ratio of the structural phase duality as shown in Fig. 1 will become very useful.

References

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Figures

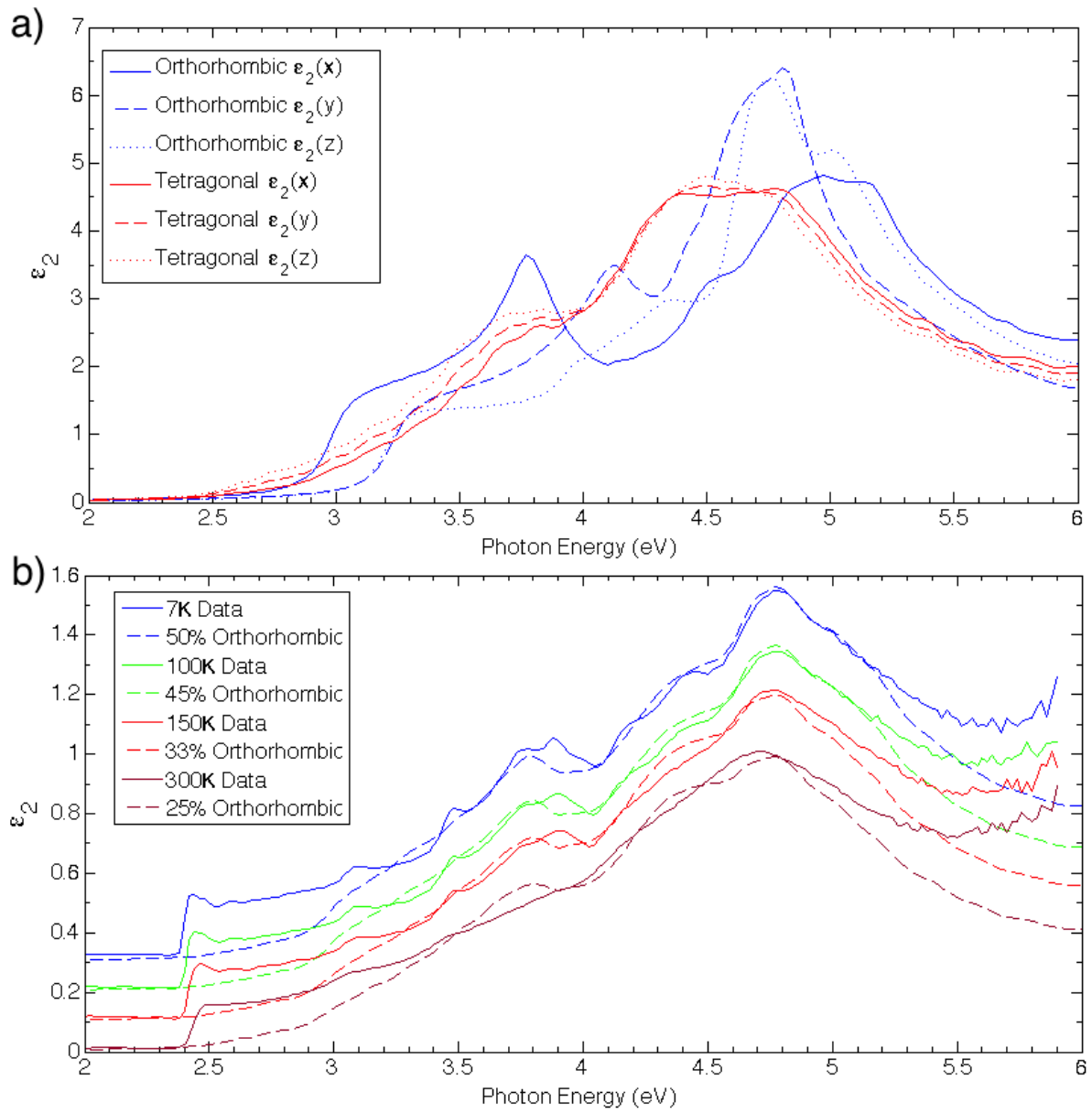

Figure 1: a The x, y and z components of ε_2 calculated from the tetragonal and the orthorhombic band structures. **b** Comparison of the combined tetragonal and orthorhombic ε_2 in different ratios with the data at 7K, 100K, 150K and 300K. Results are offset by 0.1 units for clarity.