Density of States and X-Ray Absorption Spectra of Eu-Doped Sulphides

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Abstract. Alkaline earth sulfides such as CaS and SrS are important test materials for studying the physical mechanism behind the processes in light-emitting diods (LEDs). A detailed understanding of electronic and spectroscopic properties of both clean and rare-earth-doped sulfides is thus desirable. We focus on two aspects: (i) difference between electronic structure of Eu-doped CaS and and Eu-doped SrS (in particular, also as concerns the temperature effects) and (ii) comparison of theoretical x-ray absorption spectra of CaS at the Ca K-edge and S K-edge obtained via different computational schemes with experiment.