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Atomic and Electronic Structure of Cubic and Orthorhombic PbF_2

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We have carried out first principles calculations of the atomic and electronic structure for the β (cubic) and α (orthorhombic) phases of PbF_2. A comparison of the O K calculated atomic structure for the α phase and the observed room temperature structure yields insight into the origin of the super ionic transition which occurs in both phases at elevated temperatures. The calculations also suggest a possible bcc-like structure for a higher pressure (above 150 kbar) close-packed phase which has not yet been observed. The calculated electronic structure indicates that both low pressure phases may exhibit as yet unobserved luminescence due to a 1 eV gap between the valence and first core bands. In addition, the density of electronic states (DOS) for the two phases are extremely similar which leads us to conclude that the luminescence properties of the two phases must be essentially the same for perfect crystals. The observed scintillation in the α but not the β phases must therefore result from structural imperfections present in the experimental samples of the α phase.

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