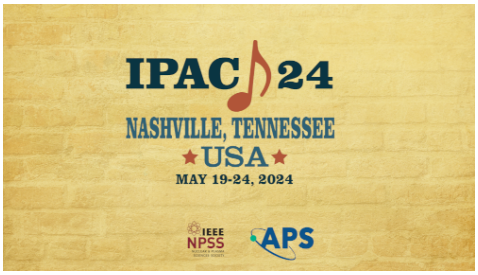

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Effects of defects on the electronic and optical properties of cesium antimonide: insights from first-principles calculations

Wednesday, 22 May 2024 16:00 (2 hours)

Cesium antimonide (Cs3Sb) photocathodes are prime candidates to replace the metallic ones currently used to generate high brightness electron beam in X-ray free electron laser and X-ray energy-recovery linacs. Their appeal stems from their outstanding photo-emissive properties, such as low work function, that give them a high quantum yield. Whereas typical computational analyses of these materials have focused on the defect-free crystal structure, the crystals grown in the laboratory are bound to have intrinsic defects that can alter their photo-emissive properties. Therefore, understanding the effect of such defects on the photo-emissive properties from first principles is essential. In this work, we started by computationally studying the effect of Cs vacancies of varying concentration on the electronic and optical properties of Cs3Sb. Our calculations reveal that such vacancies induce mid gap states in the electronic band structure. These mid-gap states lead to changes in the absorption coefficient. Such changes in the absorption coefficient suggest changes in the quantum yield of Cs3Sb, affecting its photo-emissive response.

Footnotes

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