First Principles Calculations of Iodine Vacancy Centers in SrI_2

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SrI_2:Eu^{2+} is a scintillator that has recently attracted intense interest because of its exceptional light yield and proportionality properties. However, partly because it is hygroscopic and difficult to study by routine experimental techniques, there is relatively little known of some of its properties, including lattice defects. A recent model of quenching and transport showed that linear quenching by trapping on defects as well as nonlinear quenching of dense electron-hole distributions along the primary electron track can interact with carrier transport in the track gradient to affect nonproportionality [1]. Thus information on the important lattice defects in SrI_2 is of interest for development of this material as a high-performance scintillator. We present the electronic structure and the transition energies of iodine vacancy defects in SrI_2 for several charge states. We use both semilocal (GGA-PBE) and hybrid functionals, as it is commonly accepted that hybrid functionals can improve accuracy of the band gap and hence relevant energy levels. The finite-size supercell effect is investigated in the Makov-Payne scheme [2]. Comparison, where appropriate, is made to published results on chlorine vacancy defects in NaCl calculated with similar methods and functionals [3]. Experimental searches for lattice defects and their properties in the SrI_2 family of materials are underway in Wake Forest, Fisk, Berkeley, and Livermore labs among others, and comparison to the calculations will be discussed to the extent that experimental results have become available.

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[1] Q. Li, J. Q. Grim, R. T. Williams, G. A. Bizarri, and W. W. Moses, J. Appl. Phys. **109**, 123716 (2011).

[2] Q. Makov and M. C. Payne, Phys. Rev. B **51**, 4014 (1995).

[3] W. Chen, C. Tegenkamp, and H. Pfnur, Phys. Rev. B **82**, 104106 (2010).

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