

Abstract Submitted
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***Ab-initio* Study of the Diffusion Mechanisms of Gallium in a Silicon Matrix**¹ KEVIN LEVASSEUR-SMITH, NORMAND MOUSSEAU, Département de Physique and RQMP, Université de Montréal — We present the results of a study into the diffusion mechanisms of Ga defects in crystalline Si. The dominant neutral configurations for single and multi-atom defects are established by *ab-initio* calculations using the density functional theory in the LDA approximation, with a LCAO basis as implemented in the SIESTA package. We find formation energies of 0.7 eV and 2.9 eV, respectively, for the substitutional and tetrahedral interstitial defects, while the diatomic substitutional-tetrahedral complex has a formation energy of 2.2 eV. Subsequent calculations using this same DFT package in conjunction with the activation relaxation technique (ART nouveau) allow us to determine possible diffusion pathways as well as their corresponding saddle points and energy barriers.

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