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Comparison of screened hybrid functionals to GGA functionals for predicting the properties of intrinsic radiation induced defects in Si

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Abstract content
   (Max 300 words)

The formation of radiation induced defects at room temperature can be seen to be a two-step process: Primary radiation induced defects are produced due to displacement of atoms, followed by an annealing phase during which defects relax and mobile defect species diffuse and react with each other. In order to understand the formation of radiation induced defects, it is important to understand the properties of these primary radiation induced defects.
We present defect formation and migration energies of defects calculated by DFT using GGA and hybrid functionals, and are compared to literature experimental and theoretical values. For the Si self-interstitial, using the PBEsol functional, we found that the <110>-split site was found to be the lowest energy position for the silicon self-interstitial at neutral charge state, as well as singly and doubly negative charged state. The tetrahedral site was found to be the lowest energy site for the singly and doubly charged positive states. The energy barriers for diffusion from the <110>-split site to the hexagonal and tetrahedral sites were found to be 0.370 and 0.361 eV respectively. Diffusion between the tetrahedral and hexagonal sites has an energy barrier of 0.074 eV. These energy barriers were found to be too great to account for a-thermal diffusion of the silicon self-interstitial, and diffusion paths involving cyclic changes in charge state are most likely to be responsible for the a-thermal diffusion observed at low temperature.

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Dr Walter Meyer
wmeyer@up.ac.za

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Primary author: Mr WEBB, Geoffrey (University of Pretoria)

Co-authors: Mr OUMA, Cecil (University of Pretoria); Mr PIENAAR, Jacques (University of Pretoria)

Presenter: Mr WEBB, Geoffrey (University of Pretoria)

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