Ab initio high-throughput study of extrinsic point defects in Si and Ge

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Much of initial semiconductor research was performed on Ge. End of the 1960's, interest largely shifted to Si, due to its advantages for CMOS technology. Approaching the nanoscale, Si CMOS is now reaching its physical limits. Previously problematic properties of Ge, such as the difficulty to grow stable thermal oxides are no longer relevant and the advantage of the much higher carrier mobility can be exploited.

To further explore its use, one needs a body of knowledge on Ge properties that is comparable to the one we have for Si. Given the decades of intense experimental efforts that were dedicated to Si, this is not trivial. High-throughput Density-Functional Theory calculations are one way to speed up the generation of essential knowledge on Ge properties.

The present high-throughput study focuses on one specific property: the embedding enthalpy of extrinsic point defects. This has been examined for both Si and Ge, allowing us to verify our computational method through comparison with reliable experimental data for Si, while filling in missing data for both materials. All elements from the first six periods of the periodic table (excluding lanthanides) were put at six different positions in the Si or Ge lattice. The lattice around the introduced impurity was allowed to relax. The embedding enthalpy for each impurity at each site has subsequently been determined. This approach has provided a substantial set of data for further analysis. Calculated results will be compared with available experimental data – many of those being obtained by nuclear methods (quadrupole interactions from Mössbauer, TDPAC, NMR or EPR, lattice locations studies by (emission) channeling, ...). Trends through the periodic table and the degree of transferability of knowledge for Si to the corresponding situation for Ge, will be discussed.

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