Title: Ab initio high-throughput study of extrinsic point defect embedding enthalpies in Si and Ge

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

To further explore its use, one needs a knowledge of Ge properties comparable to that of Si. Given decades of experimental efforts dedicated to Si, this is not trivial. High-throughput Density Functional Theory calculations are one way to speed up generation of essential knowledge of 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 periods one through six (excluding lanthanides) were put at six different positions in the Si or Ge lattice, which was allowed to relax. The embedding enthalpy for each impurity at each site has subsequently been determined. This approach has provided a substantial dataset for further analysis. Calculated results will be compared with available experimental data. Trends through the periodic table and the degree of transferability of knowledge for Si to the corresponding situation for Ge will be discussed.