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First-principles calculations for Er impurities in Si
LARS BJAALIE, LARS ISMER, ANDERSON JANOTTI, CHRIS G.
VAN DE WALLE, Materials Department, University of California,
Santa Barbara — Erbium-doped Si is a promising material for the de-
velopment of silicon-based light sources that can interface with CMOS
technology, optical fiber, and spin centers for quantum computing. Using
density functional theory with a screened hybrid functional we examine
the structural and electronic properties of Er(III) impurities in Si, focus-
ing on the site preference and the Er effects on the electrical properties of
the Si host. We find that Er is stable either at the tetrahedral interstitial
site or at the substitutional site, depending on the Fermi-level position;
Er sitting at the hexagonal interstitial site is higher in energy at all
Fermi levels, in agreement with experimental observations. In p-type Si,
i.e., for Fermi levels near the valence band, Er prefers the tetrahedral in-
terstitial site and acts as a donor. In n-type Si, i.e., for Fermi levels near
the conduction band, Er prefers the substitutional site and acts as an
acceptor. We will also discuss the impurity-to-band optical transitions
determined from calculated configuration coordinate diagrams.

Lars Bjaalie
Materials Department, University of California, Santa Barbara

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