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Site Preference and Electronic Properties of Erbium Defects in 4H-SiC for Quantum Emitters

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Introduction

- **Quantum emitters** are essential components of quantum networks, and solid-state defects are a promising platform.
- **Erbium in 4H-SiC** emits inside the low-loss telecom band of optical fiber in a widely available and fabrication-friendly host.
- **Problem:** There are different defect configurations erbium could have, and these different configurations have different properties.

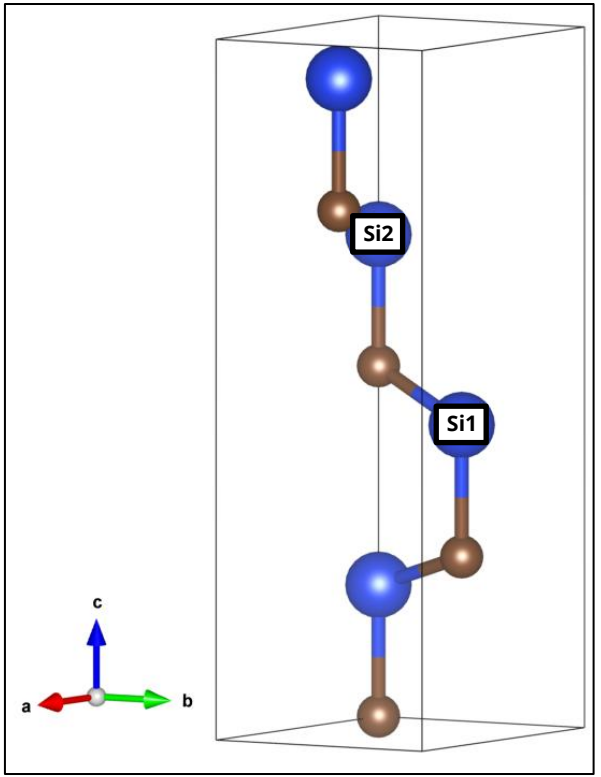

Fig. 1 | 4H-SiC unit cell with four silicon (blue) and four carbon (brown) atoms. Two silicon sites are inequivalent: quasi-cubic (k; Si1), hexagonal (h; Si2).

Methodology

- **Approach**: build many plausible erbium configurations and relax each in a 128-atom supercell.
- **Goal 1:** rank candidate configurations by formation energy (energy cost to create), identifying which defects are more likely to form.
- **Goal 2:** examine the most-likely configuration's electronic structure and charge stability.

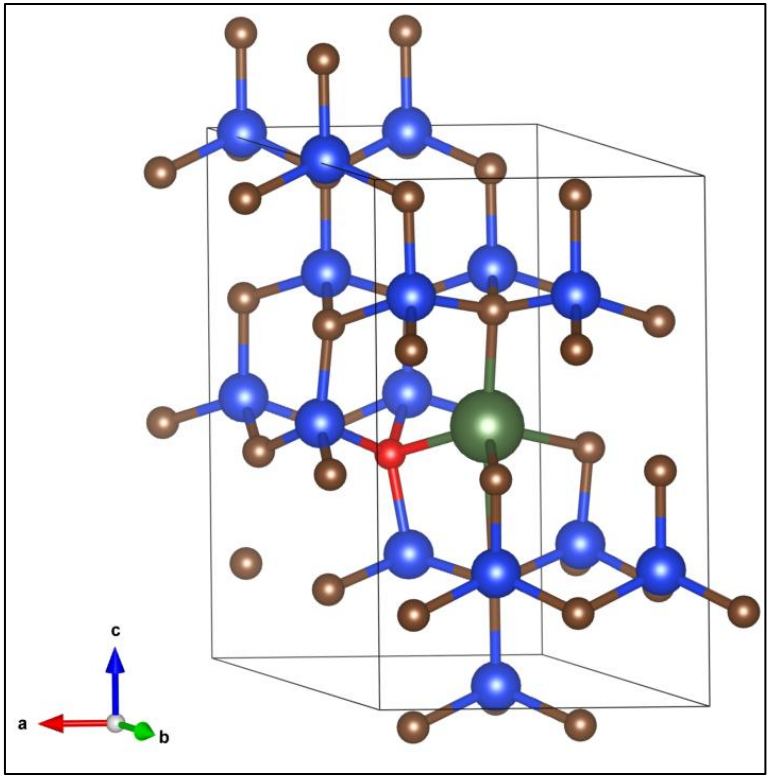

Fig. 2 | Crystal structure of $Er_{Si}(k)$ *(green)+*O_C *(red). Shown as relaxed 32-atom supercell as opposed to 128 for clarity.*

Result 1 | Site and Configuration Preference

$Er_{Si}(k)+O_C$ is the lowest-energy configuration.

Erbium-impurity complexes with O, N, P, and H are all more likely than pure substitution

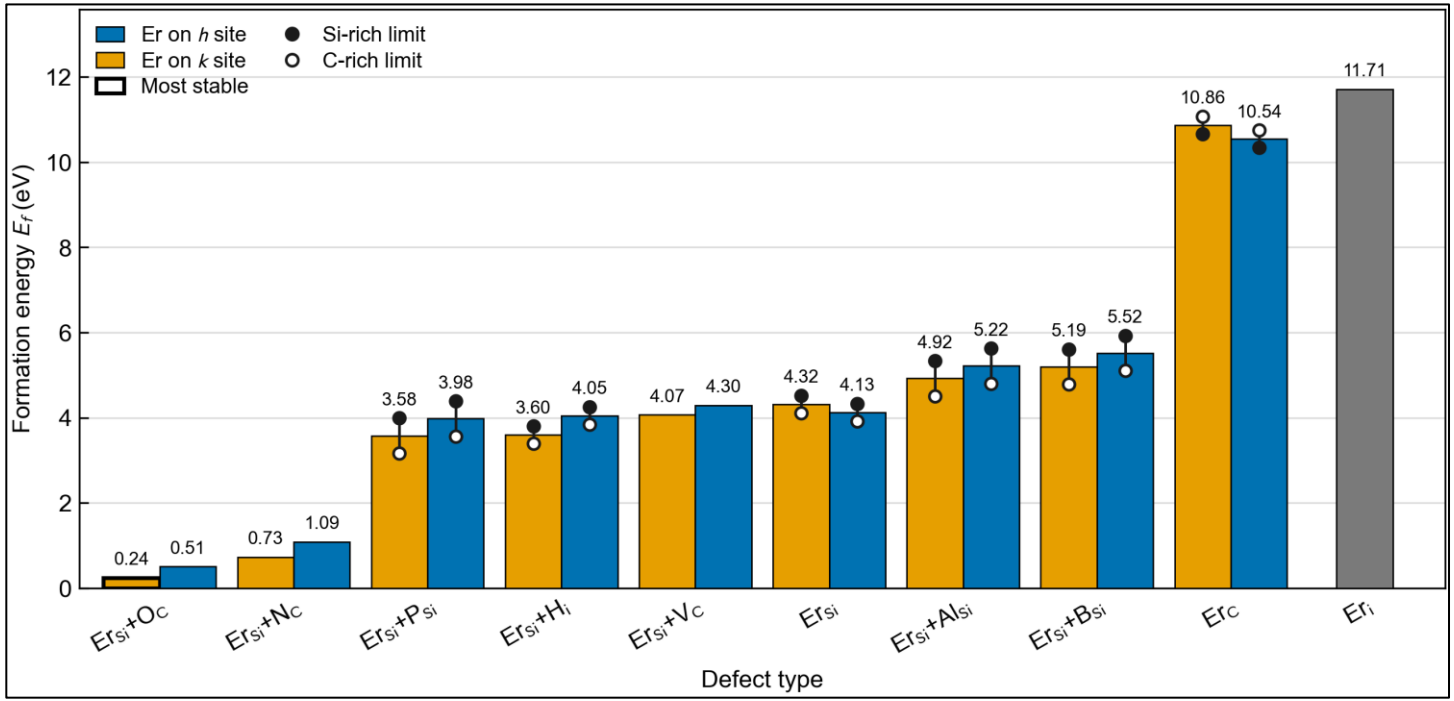

Fig. 3 | Formation energies of nineteen erbium configurations.

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Result 2 | Electronic Properties

The telecom transition from the 4f orbital stays isolated from host

+1 and neutral are the two stable charge states

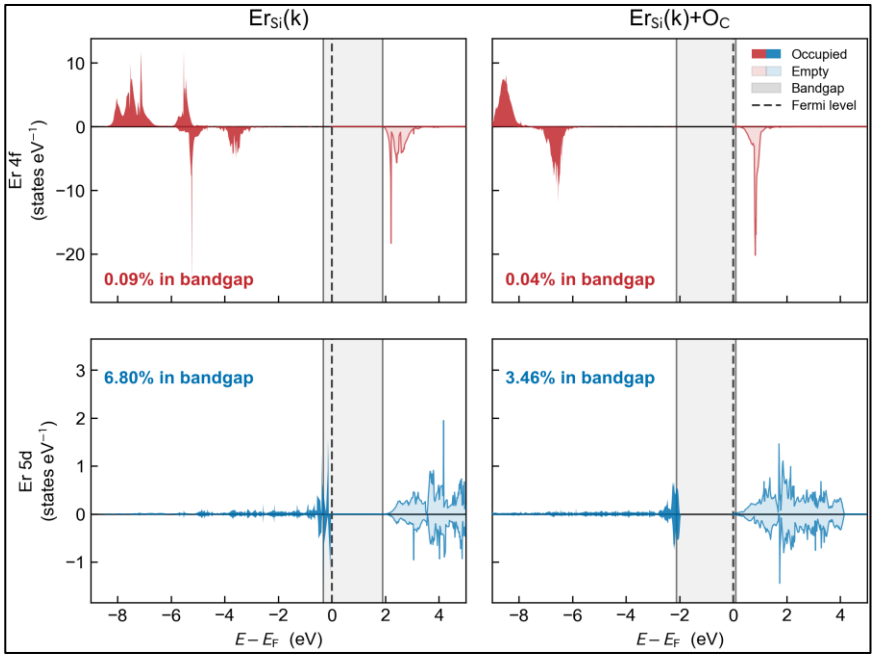

Fig. 4 | Projected DOS of isolated Er vs. the oxygen complex.

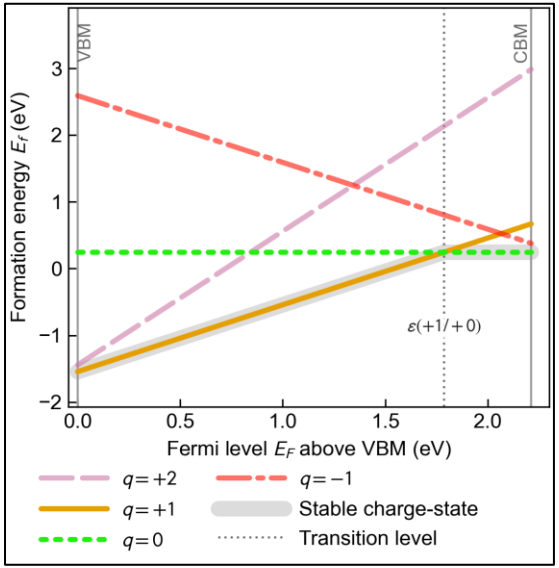

Fig. 5 | Charge-state stability.

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Discussion

- The erbium-oxygen pair is the lowest-energy configuration.
- Erbium-impurity complexes with O, N, P, and H are all more likely than pure substitution.
- The telecom transition from the 4f orbital stays isolated from host.
- +1 and neutral are the two stable charge states with a single transition in the bandgap.

These results help to identify the most likely erbium defect configurations and offer design considerations for telecom-band quantum emitters.

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Q&A

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