Calculation of complex quantum emitter defects in wide-bandgap materials

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Purpose

Color centers with active electron spin are at the heart of quantum technologies. There is a strong incentive to explore the interaction of point defects forming optically active complexes in wide-bandgap materials, for quantum communication and sensing applications.

Outline

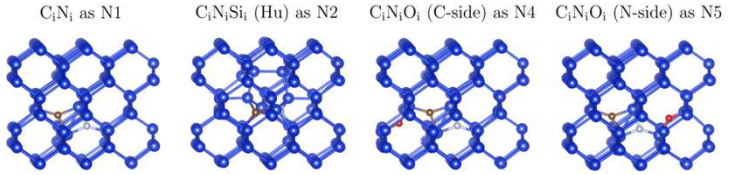
In this project, we focused on carbon-nitrogen-oxygen complex defects in silicon. Our goal was to computationally determine the atomic structure origin of the experimentally reported N-line emission series. We applied density functional theory calculations, as implemented in Quantum Espresso, to study the formation and binding properties of the defect constituents and characterize the optical transitions in the most stable complexes.

Results

We found that the neighboring interstitial nitrogen-carbon pair is a particularly stable complex in silicon and assigned it to the N1 spectral line based on its calculated optical characteristics. Interactions of this defect core with self-interstitial and oxygen interstitial defects shows reasonable agreement with further experimental lines in the N-series. These results are available in the preprint https://doi.org/10.48550/arXiv.2603.02644.

Computing system SQUID CPU

node hours	7,237
memory	156 GB/node
parallelization	4 nodes



Identified complex emitter defects in silicon.
Figure from the preprint https://doi.org/10.48550/arXiv.2603.02644.