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Formation and Annealing Behaviors of Qubit Centers in 4H-SiC from First Principles MINGWEN ZHAO, Shandong University, XIAOPENG WANG, Tulane University, HONGXIA BU, Shandong University, HONGYU ZHANG, East China University of Science and Technology, XIUJIE HE, AIZHU WANG, Shandong University, MINGWEN ZHAO'S LAB IN SHANDONG UNIVERSITY TEAM — Inspired by finding that the nitrogen-vacancy center in diamond is a qubit candidate, similar defects in silicon carbide have drawn considerable interest. However, the generation and annealing behaviors of these defects remain unclear. Using first-principles calculations, we describe the equilibrium concentrations and annealing mechanisms based on the diffusion of silicon vacancies. The formation energies and energy barriers along different migration paths, which are responsible for the formation rates, stability, and concentrations of these defects, are investigated. The effects on these processes of charge states, annealing temperature, and crystal orientation are also discussed. These theoretical results are expected to be useful in achieving controllable generation of these defects in experiments.

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