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The divacancy in SiC: A new solid-state qubit LUKE GORDON, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The nitrogen-vacancy center in diamond has attracted interest due to promising applications as a room-temperature solid-state qubit (the basic unit of a quantum computer). It is, however, desirable to identify defects that possess similar properties, but in alternative semiconductors that are either cheaper or more technologically mature. One notable defect system is the divacancy in 4H-SiC, which has recently been the subject of extensive experimental investigation. In this work, we employ advanced computational methods, particularly density functional theory using a hybrid functional, to investigate the stability and excitation energies of multiple forms of the divacancy in the various polytypes of silicon carbide. The hybrid functional gives band gaps and lattice parameters that are in excellent agreement with experiments. This allows for quantitative predictions of defect levels and zero-phonon line energies for excitation and emission processes, aiding in experimental identification of these defects.

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