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First principles identification of divacancy configurations in 4H- and 6H-SiC ADAM GALI, Wigner Research Centre for Physics, Hungarian Academy of Sciences, VIKTOR IVÁDY, Linköping University, KRISZTIÁN SZÁSZ, Wigner Research Centre for Physics, Hungarian Academy of Sciences, IGOR. A. ABRIKOSOV, ERIK JANZÉN, Linköping University — Based on the combination of ab initio simulations and group theory considerations it was proposed earlier that the high spin divacancy defect in silicon carbide (SiC) with similar electronic structure as the NV center in diamond could be utilized as a solid state quantum bit [1]. Recent demonstrations have shown coherent manipulation of divacancy and related defect spins in 4H- [2], 6H- and 3C-SiC [3]. In hexagonal SiC polytypes, point defects can exist in numerous different configurations. Associating potentially interesting photoluminescence (PL) centers with their microscopic configurations is of great importance as quantum information applications often require single defect control. In our study, we carry out large-scale first principles calculation to identify the aforementioned divacancy related point defects. By resolving accuracy issues of ab initio supercell techniques, we were able to obtain convergent PL energies, zero-field-splitting, and hyperfine parameters. Our results confirm pervious assignment of the divacancy related PL1-PL4 PL lines in 4H-SiC to their microscopic structure, provide the identification of QL1- QL6 PL lines in 6H-SiC, as well as propose defect configurations for the unknown PL5-PL6 centers in 4H-SiC that yields strong signal at room temperature. [1] A. Gali et al., Mater. Sci. Forum 645-648, 395 (2010). [2] W. F. Koehl et al., Nature 479, 84 (2011). [3] A. L. Falk et al., Nature Commun. 4, 1819 (2013).

Adam Gali
Wigner Research Centre for Physics, Hungarian Academy of Sciences

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