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Activation of dopants in SiC: theoretical study OLEG PANKRATOV, MICHEL BOCKSTEDTE, ALEXANDER MATTAUSCH, University Erlangen-Nürnberg — The electrical activation and solubility of dopants are the limiting factors that hamper the manufacturing of a highly doped SiC. In nitrogen-doped SiC a complete electrical activation was achieved [1, 2] only for impurity concentration below $2 - 5 \times 10^{19}\mathrm{cm}^{-3}$. Yet for phosphorus a full activation was obtained [1] up to $10^{20}\mathrm{cm}^{-3}$. We study the different activation behavior of these dopants theoretically by an *ab initio* DFT approach. We find that phosphorus mainly substitutes for silicon, whereas nitrogen is incorporated exclusively into the carbon sites. In a thermodynamic equilibrium the activation of both donors is not limited by the self-compensation. Phosphorus is found to be fully activated until the onset of precipitation. In contrast, nitrogen preferentially incorporates in the neutral nitrogen-vacancy complexes at concentrations above $2 \times 10^{19}\mathrm{cm}^{-3}$. This leads to the nitrogen passivation, in agreement with the experimental findings [1,2].

[1]M. Laube *et al*, J. Appl. Phys. **91**, 549 (2002).
[2]D. Schulz *et al*, Mat. Sci. Forum **338-342**, 87 (2000).

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