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Designing shallow donors in diamond¹

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The production of *n*-type semiconducting diamond has been a long-standing experimental challenge. The first-principles simulation of shallow dopants in semiconductors has been a long-standing theoretical challenge. A desirable theoretical goal is to identify impurities that will act as shallow donors in diamond and assess their experimental viability. I will discuss this identification process for the LiN₄ donor complex. It builds a scientific argument from several models and computational results in the absence of computational tools that are both trustworthy and computationally tractable for this task. I will compare the theoretical assessment of viability with recent experimental efforts to co-dope diamond with lithium and nitrogen. Finally, I discuss the computational tools needed to facilitate future work on this problem and some preliminary simulations of donors near diamond surfaces.

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