Dopants and defects in diamane films: structural details and electronic structure

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We use density-functional-theory based simulations to investigate the electronic structure of diamane films. These are thin diamond films of 2-3 layers, terminated with hydrogen atoms, which are expected to have exceptional mechanical, thermal, and electrical properties. To unravel and understand these properties we quantum-mechanically model double-layered diamane films and are specifically interested in the effect of dopants and defects on these properties. We use boron and nitrogen atoms as dopants and study also nitrogen-vacancy defects in diamane. These defects in crystalline diamond have enormous possibilities in quantum computing. Here, we address the question, whether these defects in diamane could enhance their potential as qubits. The way defects and dopants can be used to tune the electronic properties of diamane nanostructures is investigated in detail. The structural differences in these diamane structures are investigated and mapped to their electronic properties. The implications of our results in practical applications are discussed in terms of the differences in the electronic structure of diamane films as imposed by the presence of dopants and defects.