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Electronic structure properties of deep defects in hBN PRATIBHA DEV, Department of Physics and Astronomy, Howard University, PRDM COLLABORATION[1] — In recent years, the search for room-temperature solid-state qubit (quantum bit) candidates has revived interest in the study of deep-defect centers in semiconductors. The charged NV-center in diamond is the best known amongst these defects. However, as a host material, diamond poses several challenges and so, increasingly, there is an interest in exploring deep defects in alternative semiconductors such as hBN. The layered structure of hBN makes it a scalable platform for quantum applications, as there is a greater potential for controlling the location of the deep defect in the 2D-matrix through careful experiments. Using density functional theory-based methods, we have studied the electronic and structural properties of several deep defects in hBN. Native defects within hBN layers are shown to have high spin ground states that should survive even at room temperature, making them interesting solid-state qubit candidates in a 2D matrix.

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