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Interplay of Vacancy Defects and Magnetism in Carbon Structures YIMING ZHANG, SAIKAT TALAPATRA, SWASTIK KAR, ROBERT VAJTAI, SAROJ NAYAK, PULICKEL AJAYAN, Rensselaer Polytechnic Institute — Magnetic properties of diamond and graphite with vacancy defects have been studied using spin-polarized plane-wave basis density functional theory. Various scenarios of vacancy defects are investigated in these two allotropic configurations. The calculation shows that the vacancy defect concentration and nearby bonding structure is critical to determine the induced magnetism. The total magnetism start to decrease after vacancy accumulation reach the interacting configuration, in both diamond and graphite. We also shows that foreign species like nitrogen close to the vacancy is able to further enhance the magnetic moment in graphite.

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