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Study of near surface Nitrogen vacancy center (NV^-) neutralization in diamond[1] ABU NAIM RAKIB AHMED, ARTHUR NEWELL, DONTRAY DOWDELL, DEBORAH SANTAMORE, Delaware State Univ — The performance of nitrogen vacancy based sensors strongly depends on the population of NV^- near the diamond surface. The magnetic sensing capabilities of NV^- diamonds are diminished as the NV^- becomes neutralized and turns into NV^0, where NV^0 represents the neutralized charge state of NV^-. A theoretical calculation is performed to obtain the electron transfer rate between the NV^- and surface molecules using the Marcus theory of electron transfer where reorganization energy and electronic wave function coupling are considered. The electronic wave function coupling is determined using the density functional theory method. Band structure simulation is also performed to confirm the NV^- neutralization at the surface due to surface termination. The electron transfer rate is investigated for various surface terminations (hydrogen, oxygen). Moreover, an investigation of the stability of the NV^- at different depths relative to the surface is conducted. This work provides the ratio of NV^- to (NV^0+NV^-) at equilibrium, which demonstrates the effect of surface termination and contamination on NV^- neutralization and also depicts surface properties of NV^- diamonds.

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