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Anhydrous crystals of DNA bases are wide gap semiconductors.

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Abstract

We present the structural, electronic, and optical properties of anhydrous crystals of DNA nucleobases (guanine, adenine, cytosine, and thymine) found after DFT (Density Functional Theory) calculations within the local density approximation, as well as experimental measurements of optical absorption for powders of these crystals. Guanine and cytosine (adenine and thymine) anhydrous crystals are predicted from the DFT simulations to be direct (indirect) band gap semiconductors, with values 2.68 eV and 3.30 eV (2.83 eV and 3.22 eV), respectively, while the experimentally estimated band gaps we have measured are 3.83 eV and 3.84 eV (3.89 eV and 4.07 eV), in the same order. The electronic effective masses we have obtained at band extremes show that, at low temperatures, these crystals behave like wide gap semiconductors for electrons moving along the nucleobases stacking direction, while the hole transport are somewhat limited. Lastly, the calculated electronic dielectric functions of DNA nucleobases crystals in the parallel and perpendicular directions to the stacking planes exhibit a high degree of anisotropy (except cytosine), in agreement with published experimental results.

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