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Blue luminescence and the Zn acceptor in GaN: test case for the hybrid functional approach DENIS DEMCHENKO, MICHAEL RESHCHIKOV, Virginia Commonwealth University — We present a comparison of exchange tuned hybrid density functional calculations with experimental data obtained for the Zn acceptor in GaN. Since this acceptor is one of the few reliably identified defects in GaN, we use Zn-doped GaN as a test case for the widely used HSE06 hybrid functional method of calculations of defect properties in semiconductors. Here, we present the experimental results of luminescence measurements in Zn-doped GaN from which we obtain Zn acceptor defect levels. They are compared with theoretically calculated defect thermodynamic and optical transition levels, as well as the zero phonon line associated with this acceptor. We also analyze the dependence of the results on the exchange tuning procedure used in HSE06 hybrid functional. Excellent agreement with experiment is obtained when the amount of exact exchange in HSE06 is tuned to reproduce the GaN experimental band gap. This favorable comparison with the experimental results for a well-established defect suggests that the exchange tuned HSE06 hybrid functional yields accurate defect properties in GaN and therefore has significant predictive power.

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