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**Calculation of the optical properties of the nitrogen-vacancy center in diamond** DENIS ANTONOV, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany, JÖRG WRACHTRUP, 3rd Institute of Physics, University of Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany, GABRIEL BESTER, Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — We calculate the optical properties of extended and nanoscale diamond structures with embedded nitrogen-vacancy centers (NV). In particular, the negatively charged $NV^-$ center is a promising candidate for the manipulation of quantum states, quantum processing [1] and high resolution magnetometry [2]. For these applications a precise prediction and understanding of the optical properties of $NV^-$ centers and of coupled $NV^-$ centers, which are less than 10 nm apart, is required. For this task, we derive spin-polarized atomic effective pseudopotentials (AEPs [3]), which deliver results with DFT quality, but allow us to treat the large number of atoms required for the calculation of coupled NV centers. The ensuing wave functions are used in a configuration interaction approach to obtain the correlated excitonic spectra. Our results for the single defect centers are in good agreement with earlier theoretical reports [4]. The experimental zero phonon line (ZPL) and the band gap of the diamond system were reproduced with an error of 0.5%. [1] Bermudez et al., Phys. Rev. Lett. **107**, 150503 (2011) [2] Zhao et al., Nature Nanotechnology **7**,657-662 (2012) [3] J. R. Cárdenas and G. Bester, Phys. Rev. B **86**, 115332 (2012) [4] Gali et al., Phys. Rev. B

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