The bound-hole state of the NV- center in diamond

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Nitrogen-vacancy (NV) centers in diamond is a promising architecture for quantum sensing/ microscopy, quantum communications and quantum computing [1, 2, 3]. While this defect has been extensively studied [4], the charge dynamics of the NV center are one of the few aspects of this defect that are not yet fully understood. Resolving this remaining issue is key to improving the performance of the centre in its various quantum technologies and, indeed, may lead to new innovations, such as the mediation long-range coupling of NV centres by Rydberg-like states in scalable quantum computing devices [5]. Additionally, there has been a recent work observing charge transport between NV centers and the giant carrier capture cross-sections for holes [6].

In this work, we introduce a semi-ab initio method for modelling the bound-hole states of deep defects in semiconductors such as the bound-hole states of the negatively-charged NV center (NV-). Such loosely bound states are challenging to simulate because they are dispersed over several nanometers, and thus they cannot be be directly simulated by density functional theory (DFT) methods. Our approach has been to use DFT calculations to construct accurate potentials for an effective-mass model of the bound states. Solution of the effective-mass equations reveals the rich structure of the bound-hole states. We then present the first attempt at constructing a photoionization spectrum and estimating the non-radiative liftetimes and capture rates of the bound-hole states of NV-. Our semi-ab initio approach can be readily adapted to other deep defects in semiconductors.

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