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Oxygen-Boron Vacancy Defect in Cubic Boron Nitride: A Diamond NV^- Isoelectronic Center TESFAYE ABTEW, WEIWEI GAO, University at Buffalo, State University of New York, XIANG GAO, Beijing Computational Science Research Center, YIYANG SUN, SHENGBAI ZHANG, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, PEIHONG ZHANG, University at Buffalo, State University of New York — The promises of $NV^?$ center in diamond for quantum information application have inspired unprecedented research interests in optical manipulations of defect states, and have stimulated the search for alternative isoelectronic defect systems. In this talk, we present a diamond NV^- like color center in *c*-BN based on first-principles electronic structure calculations using the Heyd-Scuseria-Ernzerhof hybrid functional. The defect consists of an substitutional oxygen and an adjacent boron vacancy ($O_N{-}V_B$). We discuss the electronic and optical properties of this center in comparison with the NV- center GC-2 defect center in c-BN. We acknowledge the computational support provided by the Center for Computational Research at the University at Buffalo, SUNY. This work is supported by the US Department of Energy under Grant No. DE-SC0002623 and by the National Science Foundation under Grant No. DMR-0946404. Work at Beijing CSRC is supported by the National Natural Science Foundation of China (Grant No. 11328401).

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