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BSE calculations of color center defects in diamond[1] S. VIMOLCHALAO, U. of Washington, W.H. LIANG, UC Merced, F.D. VILA, J.J. KAS, J.J. REHR, U. of Washington, F. FARGES, Muséum National d'Histoire Naturelle, Paris — Colored diamonds are both of fundamental and commercial interest. Several recent efforts have focused on determining the origin of their color. For example, experiments show that the color of blue diamonds is associated with isolated boron impurities[2] while nitrogen impurities are responsible for yellow diamonds. It has previously been shown [3] that theoretical Bethe-Salpeter Equation (BSE) simulations of boron-doped diamond yield a dark-blue diamond in good agreement with that observed. However, the structure of the nitrogen defects is not well understood. Here we present BSE calculations of the optical response of nitrogen-doped diamonds using relaxed 64-atom unit cells. We focus on N_xV_y defect sites, where x is the number of substitutional nitrogen atoms and y is the number of carbon vacancies. We find that the most likely candidates are the N_3V_1 and N_2V_0 defects, which show absorption in the 2.5-3.2 eV range, consistent with yellow color. Our results also rule out the N_1V_0 and N_4V_1 defect types as possible yellow centers.

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[2]J.Walker, Rep. Prog. Phys. **42** 1605 (1979).
[3]F.Farges *et al.*, Europhysics News **43**, 20 (2012).

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