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Role of native defects and related complexes in absorption and luminescence of AlN[1] QIMIN YAN, ANDERSON JANOTTI, Materials Department, University of California at Santa Barbara, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, CHRIS G. VAN DE WALLE, Materials Department, University of California at Santa Barbara — AlN is a wide-band-gap material that has being considered as a substrate for GaN-based optoelectronic devices, or in its own right for deep ultraviolet light-emitting diodes and laser diodes. The band gap of 6.2 eV in principle allows transparency in the visible to UV range, but in practice AlN crystals exhibit several sub-band-gap absorption and emission bands, likely due to the presence of native defects and impurities (the most common being oxygen). Using first-principles calculations with the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE), we investigate the structural, electronic, and optical, properties of N and Al vacancies, and their complexes with O impurities in AlN. Defect charge transition levels and stable charge states are determined from the calculated formation energies, and absorption and emission energies are obtained by constructing configuration coordinate diagrams. Our results indicate that Al vacancies and O impurities are responsible for several absorption/emission lines observed experimentally, in particular for the absorption band around 2.85 eV (which gives AlN crystals a yellowish color) and the emission around 3.20 eV emission (375 nm), often observed in O-doped AlN. Mechanisms for each of these processes will be discussed in detail.

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