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Why nitrogen cannot lead to p-type conductivity in ZnO[1] JOHN L. LYONS, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Nitrogen is often considered as the most suitable dopant for achieving p-type ZnO since it has a similar size to oxygen and has successfully been used as a shallow acceptor in ZnSe. In spite of many published reports on p-type ZnO achieved by nitrogen doping, reproducibility and stability still seem to be major issues, and devices based on pn junctions have remained elusive. We have studied the electronic and structural properties of the nitrogen acceptor in ZnO using state-of-the-art first-principles calculations based on hybrid functionals (Heyd-Scuseria-Ernzernhof). We find the nitrogen acceptor level to be 1.3 eV above the valence-band maximum. Nitrogen therefore cannot lead to hole conductivity in ZnO. We have analyzed the optical properties (absorption and luminescence), which should offer characteristic experimental signatures of nitrogen in the lattice. Previous experimental reports are discussed in light of our new results.

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John L. Lyons
University of California, Santa Barbara

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