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Substitutional hydrogen as a cause of the unintentional n-type conductivity in ZnO. ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara, CA 93106-5050 — ZnO is a wide-band-gap semiconductor that is very promising for optoelectronic device applications. Serious challenges remain, however, and controlling the electrical conductivity is the most fundamental among these. As-grown ZnO is n-type and the cause of this n-type conductivity is still widely debated. Oxygen vacancies have long been invoked as the source of the n-type conductivity. This assignment is based on the assumption that oxygen vacancies are shallow donors, and on the fact that the conductivity changes inversely with the oxygen partial pressure. Contrary to the conventional wisdom, we have recently established that oxygen vacancies are not shallow but deep donors and have high formation energies in n-type ZnO. Therefore, they cannot cause conductivity. Based on first-principles calculations we show that SUBSTITUTIONAL hydrogen is a likely cause of the unintentional conductivity in ZnO. Hydrogen on an oxygen site forms a multicenter bond. Substitutional hydrogen is a shallow donor, and has a migration barrier of 2.5 eV, explaining recent observations of a hydrogen-related donor that is stable up to 500 ^{o}C.

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