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Influence of the "second gap" on the optical absorption of transparent conducting oxides VIET-ANH HA, DAVID WAROQUIERS , GIAN-MARCO RIGNANESE , GEOFFROY HAUTIER , Institut de la matière condensée et des nanosciences (IMCN), Université catholique de Louvain, Louvain-la-Neuve 1348, Belgium — Transparent conducting oxides (TCOs) are critical to many technologies (e.g., thin-film solar cells, flat-panel displays or organic light-emitting diodes). TCOs are heavily doped (n or p-type) oxides that satisfy many design criteria such as high transparency to visible light (i.e., a band gap $>$ 3 eV), high concentration and mobility of carriers (leading to high conductivity), ... In such (highly doped) systems, optical transitions from the conduction band minimum to higher energy bands in n-type or from lower energy bands to the valence band maximum in p-type are possible and can degrade transparency. In fact, it has been claimed that a high energy ($>$ 3eV) for any of these transitions made possible by doping, commonly referred as a high "second gap", is a necessary design criterion for high performance TCOs. Here, we study the influence of this second gap on the transparency of doped TCOs by using *ab initio* calculations within the random phase approximation (RPA) for several well-known p-type and n-type TCOs. Our work highlights how the second gap affects the transparency of doped TCOs, shining light on more accurate design criteria for high performance TCOs.

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