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**Materials for Transparent Electronics: Ab initio calculation of wide bandgap semiconductor interfaces** SKYE DORSETT, GUENTER SCHNEIDER, Oregon State University — Materials used in transparent electronics (TE) must be transparent in the visible portion of the electromagnetic spectrum which requires the use of wide bandgap semiconductors as contacts and rectifiers as well as passivation and barrier-shaping layers. Of particular importance are the source and drain contacts of transparent thin-film transistors (TTFT). The contact characteristics at the interface between the channel material (e.g. ZnO, SnO<sub>2</sub>) and the contact material (commonly Indium Tin Oxide) are determined by the band offset which can be estimated from a heterojunction model based on material properties alone. The development of new materials for TE greatly benefits from estimates of interface properties but for most materials which hold promise for use in TE (e.g. indium gallium zinc oxide) the relevant material parameters such as work function, electron affinity and in particular the charge neutrality level are not known. To close this gap we report ab-initio density functional theory calculations of band offsets for wide bandgap semiconductors which are commonly used or hold promise for use in TTFT.

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