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First-principles study of InX (X=P,Sb) semiconductors OSCAR D. RESTREPO, ROHAN MISHRA, WOLFGANG WINDL, The Ohio State University — III-V semiconductors are gaining increasing interest for applications due to the possibility of engineering their electronic properties by choosing and combining different elements. Additional design parameters can come from confinement effects which have led to intensified research on nanowires for electronic applications. Among the lesser studied III-V semiconductors with large technological potential are indium-based compounds, where InSb with an extremely small band gap in the infrared range is the staple material for infrared detector devices and InP (with a larger band gap of 1.42 eV) is considered as a promising material for nanowire-based applications. For these materials, many basic questions that have been answered for more-mainstream semiconductors are still unanswered, these include effective masses, optical properties, and the influence of defects on their properties. In order to address some of these questions, we have performed an exhaustive exploration of the defect energetics of InP using first-principles calculations. We also report a detailed comparison of calculated effective masses and optical properties of InSb with experiments. We have used both GGA and HSE06 to treat exchange-correlations. This work was supported by NSF MRSEC DMR-0820414.

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[X] Prefer Oral Session
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