Structural, electronic and phononic properties of two-dimensional InBr, InI, TlCl and TlBr

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The indium and thalium monohalides are semiconductors that are known as a mercury free alternative in plasma lighting applications. Lately, layered material surfaces are focus of attention due to possible applications in novel optoelectronic devices, and the reported electronic properties of thalium and indium monohalides are extremely promising on this regard [1-4]. To increase the knowledge of such surfaces, we investigate the structural, electronic and phononic properties of two-dimensional InBr, InI, TlBr and TlCl by performing first principles electronic structure calculations. Our calculations indicate that monolayers of these structures can be cleaved from their bulk forms straightforwardly using readily available cleaving methods. We report surface bands with a direct energy band gap in the visible range: 2.48 eV for InBr, 2.28 eV for InI, 2.85 eV for TlBr and 3.26 eV for TlCl. We also report the red shift in Raman active modes going from bulk to monolayer phases in InBr, InI, TlBr and TlCl. A property of particular interest for optical applications is the reported sensitivity of the quasiparticle bands to the biaxial tensile stress in bulk. We report this effect is also present at the cleaved surface, and surface conduction band minimum near the X or the Y point in BZ and bandgap slightly increases under tensile stress.

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References:
[1] A. Borghesi, G. Guizzetti, L. Nosenzo, E. Reguzzoni, A. Stella, and F. Lévy. Solid State Communications 48 (4), 345-348 (1983).
[2] J. Wang, B. Dong, H. Guo, T. Yang, Z. Zhu, G. Hu, R. Saito, and Z. Zhang, Physical Review B, 95(4), 045404 (2017).
[3] H. C. J. Mulders, A. J. Rijke, M. Haverlag and G. M. W. Kroesen, Journal of Physics B: Atomic, Molecular and Optical Physics. 44 (14) 145101 (2011).
[4] T. Low, A. Chaves, J. D. Caldwell, A. Kumar, N.X. Fang, P. Avouris, T. F. Heinz, F. Guinea, L. Martin-Moreno, F. Koppens, Nature Materials 16(2), 182-194 (2017).