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Band gap formation in tetrahedrally bonded I_3-V-VI_4 semiconductors-the role of V lone pairs[1] S.D. MAHANTI, DAT DO, Department of Physics, Michigan State University — An interesting class of tetrahedrally coordinated ternary compounds have attracted considerable interest because of their potential as good thermoelectrics. These compounds, denoted as I_3-V-VI_4, contain three monovalent-I (Cu, Ag), one pentavalent-V (P, As, Sb, Bi), and four hexavalent-VI (S, Se, Te) atoms; and can be visualized as ternary derivatives of the II-VI zincblende or wurtzite semiconductors, obtained by starting from four unit cells of (II-VI) and replacing four type II atoms by three type I and one type V atoms. In trying to understand their electronic structures and transport properties, some fundamental questions arise: whether V atoms are indeed pentavalent and if not how do these compounds become semiconductors, what is the role of V lone pair electrons in the origin of band gaps, and what are the general characteristics of states near valence band maxima and conduction band minima. We will answer some of these questions using ab initio electronic structure calculations (density functional methods with both local and nonlocal exchange-correlation potentials). Some part of this work has been published in Dat et al, J. Phys.: Condens. Matter 24, 415502 (2012).

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S, D. Mahanti
Department of Physics, Michigan State University

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