Energies for Muonium Defect Levels in Semiconductors

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The ionization energies for donor and acceptor states of muonium have been obtained for a series of semiconductors in order to place the related thermodynamic defect levels with respect to the conduction and valence band edges. This work was initiated following a claim [1] that the Fermi level at which the equilibrium charge-state for the negative-U impurity hydrogen changes from positive to negative, the so-called H(+/t) level, should lie at a fixed energy on an absolute scale independent of host material. This level lies midway between the inverted donor H(0/+) and acceptor H(t/0) levels. Muonium quite accurately mimics the behavior of hydrogen with respect to its charge states and basic sites, thus data for Mu experimentally models the H defect levels with appropriate adjustments for the additional zero-point vibrational energy of Mu at equivalent locations. In a cubic diamond or zincblende structured material, the bond-centered (BC) location is the donor site. The acceptor is located in the tetrahedral interstitial region, centered at the T-site for Mu but probably off-center for H. Our experimental efforts have concentrated on semiconductors for which at least two neutral muonium centers are observed, thus offering the possibility of identifying both the electron and hole ionization transitions and obtaining the associated energies. We will summarize the results thus far obtained for Mu and discuss an estimate of the adjustments required to translate these defect-level energies to hydrogen. In addition to statistical uncertainties in fitting the data, the largest uncertainty associated with placement of the Mu(+/t) level is related to difficulty in obtaining the energy difference for Mu^0 located at the BC and T sites. The results generally support a common Mu(+/t) level, but place that level at a significantly higher energy than predicted for H, well outside the range of estimated zero-point energy corrections. We also obtain a value of U for Mu in each material as the energy difference between the donor and acceptor levels, to be compared with that obtained from calculated formation energies. The most important consequence for the properties of hydrogen in semiconductors is that more materials should be doped n-type by H, and fewer p-type, based on our adjusted H(+/t) level.

[1] C.G. Van de Walle and J. Neugebauer, Nature 423 (2003) 626.