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Charged defect in GaSb by selective occupation in density functional theory[1] JIANWEI WANG, YONG ZHANG, Department of Electrical and Computer Engineering, UNC Charlotte — In a density functional theory (DFT) approach, the transition energy of an acceptor-like defect is typically calculated by the total energy difference between E(N+1) and E(N), where N is the total number of the valence electrons of the defected system. Effectively, in this scheme, the hole in the valence band is simulated by a uniform positive background charge or a plane wave. A scheme closer to the reality would be to move one electron from the valence band maximum (VBM) to the defect level, because the VBM state usually is quite different from a plane wave. We apply this selective occupation scheme to a defect problem, an antisite defect of Ga on Sb in GaSb, and compare the results of two schemes with varying supercell size, using a pseudopotential DFT theory.

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