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Genuine impurity states vs. perturbed host states in a supercell approach YONG ZHANG, A. MASCARENHAS, NREL, L.-W. WANG, LBNL — The spatial localization is the most basic feature of an impurity state(IS) in a semiconductor. However, in the often used supercell approach, this feature might not be practically reliable, especially when the IS's are in resonance with the host state. We have developed a systematic approach for identifying the genuine IS's amongst the large number of states given by the supercell calculation[1], with the help of a charge-patching method that allows us to perform the electronic structure calculation with an accuracy near that of a self-consistent DFT and the ability handling >10K atoms[2]. We have applied this approach for two prototype systems: (1) isoelectronic "acceptor" in GaP:N, for which we have shown the non-existence of any excited state of N impurity in the conduction band within at least a few hundred meV proximity of the N bound state[1], in contrast to the decades old speculation and recent claim of the existence of such excited states; (2) isoelectronic "donor" in GaAs:Bi, for which we have found a resonant IS generated by Bi within the valence band (VB) and the topmost VB state is that of GaAs perturbed by Bi[3], which reveals a strong enhancement in the spin-orbit splitting (confirmed experimentally[4]) and resolves the speculations whether or not Bi could have a bound state in GaAs. [1] Zhang et al.,PRB**74**,R41201 (06). [2] Wang, PRL **88**,256402 (02). [3] Zhang et al., PRB**71**,155201 (2005). [4] Fluegel et al., PRL**97**,67205 (06). DOE/BES

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