

# Towards Fermi level De-pinning at Contacts

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Fermi level pinning at Schottky barriers (SB) strongly limits the reduction of contact resistances and thus scaling of modern electronic devices and future 2D semiconductor devices. We find that some complex semiconductor-metal interfaces with bonding configurations parallel to the interface create a type of localized interface or ‘defect state’ beyond the metal induced gap state (MIGS) model. Examples are interfaces between Si and metal disilicides and between Si and Sb. These defect states do not easily match to conventional MIGS and this mixes states of metal character into the surface pinning level. This creates Fermi level de-pinning and a variation of SB height with interface orientation.

The MIGS model [1] has successfully described many aspects of Schottky barrier behavior, including the slope of barrier height (SBH) with metal work function,  $S = \partial\phi / \partial\Phi_M$  and the charge neutrality level. However, it does not include several factors like interface bonding [2]. The MIGS model would say the  $S$  factor should depend only on metal work function, not type of metal (elemental or silicide/TiN) or on the face orientation, despite these being seen experimentally [2,3] and found in DFT supercell calculations [4]. We show that both metal silicides and Sb break the MIGS due to the presence of ‘defect-like’ states [5] at their interfaces, due to states which cannot be easily captured by the limited MIGS basis set of bulk semiconductor states. A metal-like character enters the effective CNL pinning energy, which also gives the orientation dependence. The chemically different case of Si:Sb behaves similarly to the silicides. These two factors are signifiers of Fermi level de-pinning, to find other examples.

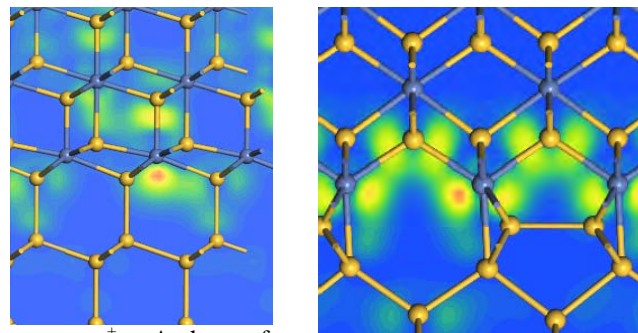
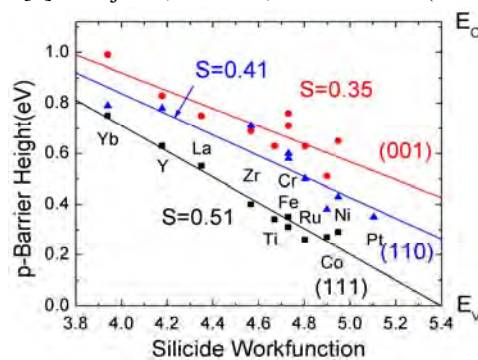
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Figure 1 Showing Fermi level depinning and face dependence in Si: silicide interfaces

Figure 2 Showing ‘defect state at Si:silicide (111), (100) interfaces causing the de-pinning and orientation dependence