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**First-principles calculations on metal-induced gap states at metal-semiconductor interfaces** Y. GOHDA, S. TSUNEYUKI, Department of Physics, The University of Tokyo, 113-0033 Japan — Metal-induced gap states (MIGS) are responsible for Fermi-level pinning for narrow-gap semiconductors such as Si and GaAs. First-principles calculations have demonstrated that MIGS are related to the tails of metal states penetrating into the semiconductor corresponding to Bloch states with wave vectors having an imaginary part. Thus, their existence is a consequence of intrinsic properties of the bulk semiconductor. In contrast, a removal of FLP has been reported experimentally at atomically controlled Al-Si(100) interfaces, suggesting that MIGS play a less dominant role in determining the interface properties. This inconsistency between experimental results and the accepted view of MIGS calls for a detailed theoretical investigation. Here, we report our recent progresses on MIGS at a few metal-semiconductor interfaces investigated by means of first-principles calculations.

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