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Schottky barrier formation and reduction at Au/TiO_2 interfaces by dopants from quantum simulations YANG JIAO, ANDERS HELLMAN, YURUI FANG, Applied Physics, Chalmers University of Technology, SHIWU GAO, Beijing Computational Science Research Center, MIKAEL KÄLL, Applied Physics, Chalmers University of Technology — Excitation of localized surface plasmon resonances (LSPRs) in metallic nanoparticles, especially particles made of noble metals, results in efficient light absorption and strong field enhancement, thereby enabling a multitude of nanooptical applications of high current interest. Recently, the possibility of utilizing LSPRs to generate hot electrons has attracted considerable attention. One method to extract and make use of the hot electrons is by attaching the nanoparticles on a semiconductor surface such that excited electrons with proper energy and momentum can be transferred through the Schottky barrier at the interface. Using *ab initio* calculations for Au/TiO_2 interfaces, we investigate dopant induced Schottky barrier height reduction effects. We show that dopant induced polarization at the interface is the dominant reason behind the semiconductor band bending and Schottky barrier formation. Calculations for Nb-dopants at different depths (d) below the interface show that the Schottky barrier height reduction depends on the depth and varies from 0.1 eV at $d = 4$ nm to up to 1.3 eV when the dopant is situated at the interfacial layer. The calculations also indicate that the Schottky barrier can be tuned by up to 1.5 eV by using different transition metal dopants.

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