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Density-Functional Calculation for the Junction between Metal and Semimetal CHIN-SHENG WU, Center for General Education, Yuan-Ze University, Nei-Li, Taiwan — . We apply the density-functional theory to calculate the junction characteristics between the metal and semimetal. We obtain the self-consistent solution of the charge distribution both when Fermi levels of the metal and semimetal are set equal and when they are set unequal. The differential junction capacitance is obtained by differentiating the areal charge density with respect to the shift of Fermi levels. The electronic structure, potential, differential junction capacitance for the interface are reported. Our calculations for the metal with the conduction electron densities r=2, 6, and 12 a.u., and the semimetal with r=24 a.u.

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