Density-Functional Calculation for the Surface of Metal Wire

CHIN-SHENG WU, Center of General Education, Yuan-Ze University, Nei-Li, Taiwan — We apply the density-functional theory to calculate the surface electron structure of metal wire. We obtain the self-consistent solution of the charge distribution around the surface. The differential surface capacitance is obtained by differentiating the areal charge density with respect to the shift of Fermi levels. The electronic structure, potential, differential surface capacitance for the cylindrical metal wires are reported. Our calculations for the metal wire with the conduction electron densities $r=2, 6, \text{ and } 12 \text{ a.u.}$ are performed.