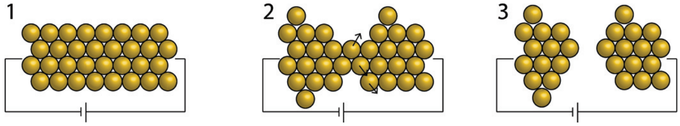
Solutions to Problems

Chapter 2

1. Examples of the three classes include (i) mechanical methods such as mechanical break junctions, atomic force microscopy or scanning tunneling microscopy; (ii) advanced nanofabrication methods such as electromigration method or advanced evaporation methods; (iii) self-assembly method, such as the assembly of nanoparticle or nanorod dimers.
2. (i) The length of typical molecules are in the order of 1–2 nm, much smaller than typical micro-fabricated structures, therefore fabrication of suitable nanoscale electrodes are a challenge.
   (ii) A second challenge is how to isolate a single and not two or more molecules in the nanogap between two or three electrodes.
   (iii) Since the molecules typically cannot be manipulated by direct means, self-assembly methods need to be developed for the molecules to assemble at the electrodes without direct human interaction.
3. A bias is applied to a thin constriction on a wire (1). As the electrons move through the wire, they scatter on the gold atoms and the momentum starts to move gold atoms (2). A nanogap is formed as the wire breaks (3).



4. From Eqs. (2.1–2.3) of the textbook, for molecule **a** we have

   $G = G_{\rm air} \exp\,(-\alpha_{\rm air}\ \mathrm{d}_1)$

   $G = G_{\rm a} \exp\,(-\beta_{\rm a}\ \mathrm{h}_{\rm a})$

   The combined tunneling of double layer of **a** and air is given by equation 2.3:

   $G_1 = G_{\rm a} \exp\,(-\beta_{\rm a}\ \mathrm{h}_{\rm a})\ G_{\rm air} \exp\,(-\alpha_{\rm air}\ \mathrm{d}_1)$

   For molecule **b** we can write an identical expression

   $G_2 = G_{\rm b} \exp\,(-\beta_{\rm b}\ \mathrm{h}_{\rm b})\ G_{\rm air} \exp\,(-\alpha_{\rm air}\ \mathrm{d}_2)$

   Since the experiment is carried out in a constant current mode, then $G_1 = G_2$ we can now combine the equations to get

   $G_{\rm a} \exp\,(-\beta_{\rm a}\ \mathrm{h}_{\rm a})\ G_{\rm air} \exp\,(-\alpha_{\rm air}\ \mathrm{d}_1) = G_{\rm b} \exp\,(-\beta_{\rm b}\ \mathrm{h}_{\rm b})\ G_{\rm air} \exp\,(-\alpha_{\rm air}$ $\mathrm{d}_2)$, which can be rewritten to

   $(G_{\rm a} G_{\rm air}/G_{\rm b} G_{\rm air})\ \exp(-\beta_{\rm a}\ \mathrm{h}_{\rm a} - \alpha_{\rm air}\ \mathrm{d}_1) = \exp(-\beta_{\rm b}\ \mathrm{h}_{\rm b} - \alpha_{\rm air}\ \mathrm{d}_2)$

   Assuming $G_{\rm a} \approx G_2$ we can reduce expression to

   $-\beta_{\rm a}\ \mathrm{h}_{\rm a} - \alpha_{\rm air}\ \mathrm{d}_1 = -\beta_{\rm b}\ \mathrm{h}_{\rm b} - \alpha_{\rm air}\ \mathrm{d}_2$, where β_b can be isolated as follows:

   $(\beta_{\rm a}\ \mathrm{h}_{\rm a} + \alpha_{\rm air}\ (\mathrm{d}_2 - \mathrm{d}_1))/\ \mathrm{h}_{\rm b} = \beta_{\rm b}$

Chapter 3

1. We assume a small symmetric voltage drop V over the junction. At zero temperature, the Fermi functions in left (L) and right (R) leads are reduced to step functions

   $$\phi_{L/R}(\varepsilon) = \frac{1}{1 + e^{(\varepsilon - \mu_{L/R})/k_{\rm B}T}} \to \Theta\left(\frac{\varepsilon - \mu_{L/R}}{k_{\rm B}T}\right) \tag{3.1}$$

   with $\mu_{L/R} = E_F \pm eV/2$. Eq. (3.35) of the textbook then reduces to

   $$\mathcal{J} = \frac{2e}{h}\int_{E_F - eV/2}^{E_F + eV/2} T(\varepsilon)\, d\varepsilon \tag{3.2}$$

   with the transmission function given by

   $$T(\varepsilon) = \frac{4\mathrm{Im}[\Gamma_R^R]\mathrm{Im}[\Gamma_L^R]}{(\varepsilon - \tilde{E})^2 + (\mathrm{Im}[\Gamma_\Sigma^R])^2}. \tag{3.3}$$