Band bending in contact between physiological salt solution and ZnO or Cu_2O semiconductor

M. Pławecki[1], E. Rówiński[1]

[1] *Institute of Materials Science, University of Silesia, 75 Pułku Piechoty Street 1A, Chorzów, Poland*

When a semiconductor comes into contact with a liquid (redox species), to maintain electrostatic equilibrium, there will be a charge transfer between the n-type or p-type semiconductor and liquid phase if formal redox energy level of redox species lies inside semiconductor band gap [1,2,3,4,5]. We have considered one dimensional particle energy bands for the nearly free particle model at a physiological salt solution/semiconductor interface. With the help of Schrodinger equation and Bloch's theorem, it is possible to formulate a general approach to derive both the band bending and direct band gap in the interface. The Bloch's theorem shows that translational symmetry in real space leads to translational symmetry in k-space. For simplicity the model was introduced to account for the effects of band bending at the interface. Band diagram of two occupied and unoccupied bands separated by the energy gap at the semiconductor (before contact) and the interface (after contact) is illustrated in Figure 1. The model produces the correct band bending structure of physiological salt solution/n-type ZnO semiconductor and physiological salt solution/p-type Cu_2O semiconductor interfaces.

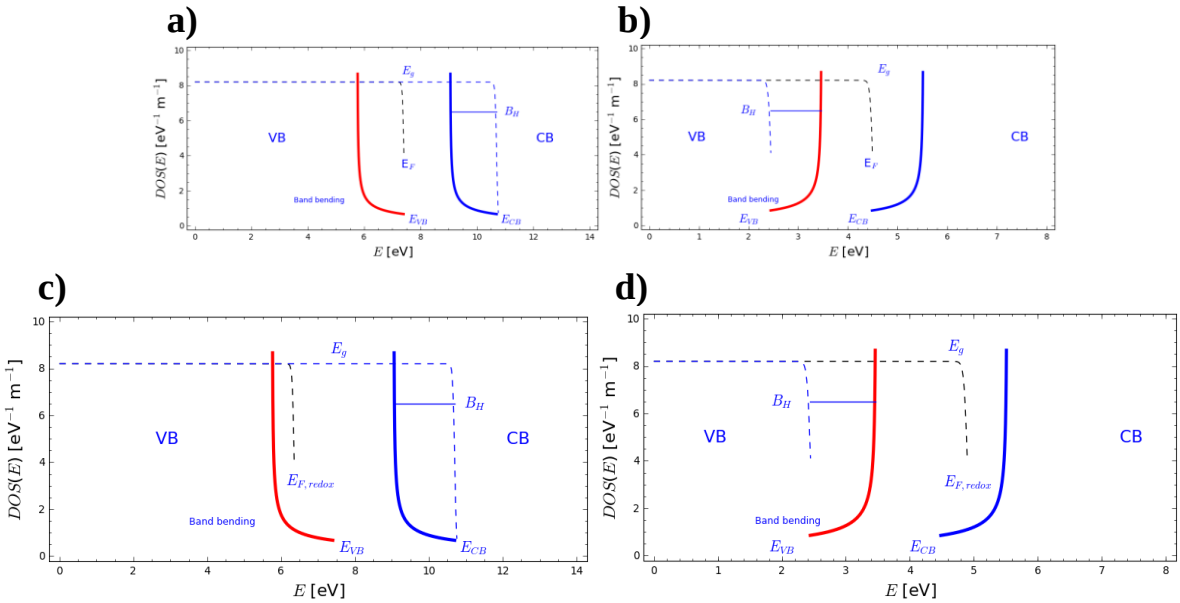

Figure. 1 The density of states in various types of materials: **a)** ZnO **b)** Cu_2O **c)** the 5 µL physiological salt solution/ZnO semiconductor interface **d)** the 5 µL physiological salt solution/Cu_2O semiconductor interface. DOS(E) denotes the density of states, and E_{VB} is the maximum energy of the valence band, E_{CB} is the characteristic energy of the conduction band and B_h is the energy barrier height. E_g is the energy gap, E_F is the Fermi level of semiconductors (before contact), $E_{F,redox}$ is the redox Fermi level of interfaces (after contact).

[1] Z. Zhang, J. T. Yates, Chem. Rev. **112**, 5520 (2012).
[2] A.J. Bard, A.J. Bocarsly, J. Am. Chem. Soc. **102**, 3671 (1980).
[3] E. Rówiński, M. Pławecki, Acta Physica Polonica A **130/4**, 1141 (2016).
[4] M. Pławecki, E. Rówiński, Ł. Mieszczak, Acta Physica Polonica A **130/4**, 1144 (2016).
[5] M. Pławecki, B. Bzowski, A.T. Trycz, E. Rówińskiar, Xiv:1609.08361 [cond-mat.mtrl-sci]