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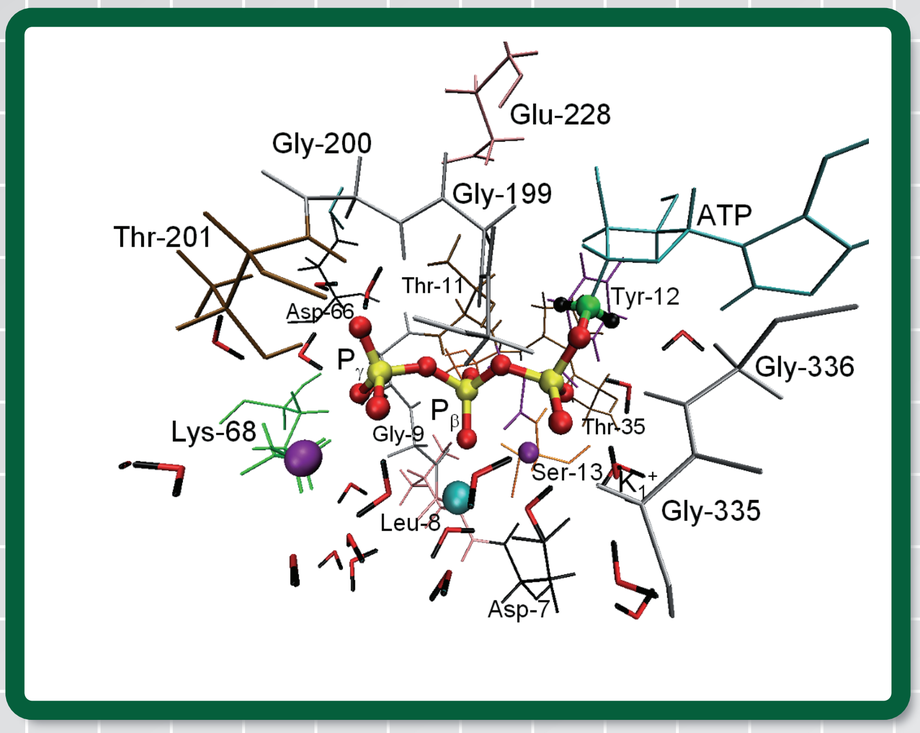
Computational Material and Life Sciences I

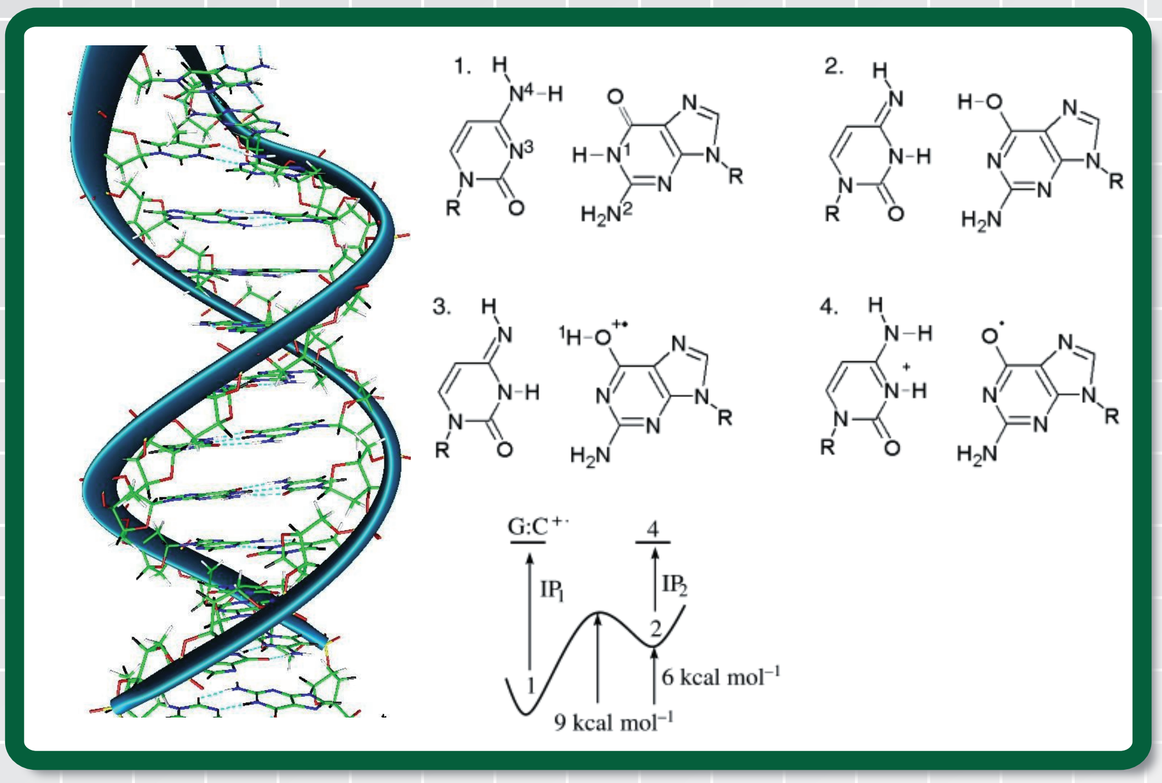
ATPase in Hsc70 protein

QM/M simulations, coupled to metadynamics, on Hsc70 ATPase protein, show how a water molecule coordinated to Mg^{2+} acts as a catalyst and evidence the unique and cooperative role of K^+ and Mg^{2+} metal ions in promoting the release of the inorganic phosphate via an exchange of OH^- between their respective solvation shells.



Charge transfer in DNA

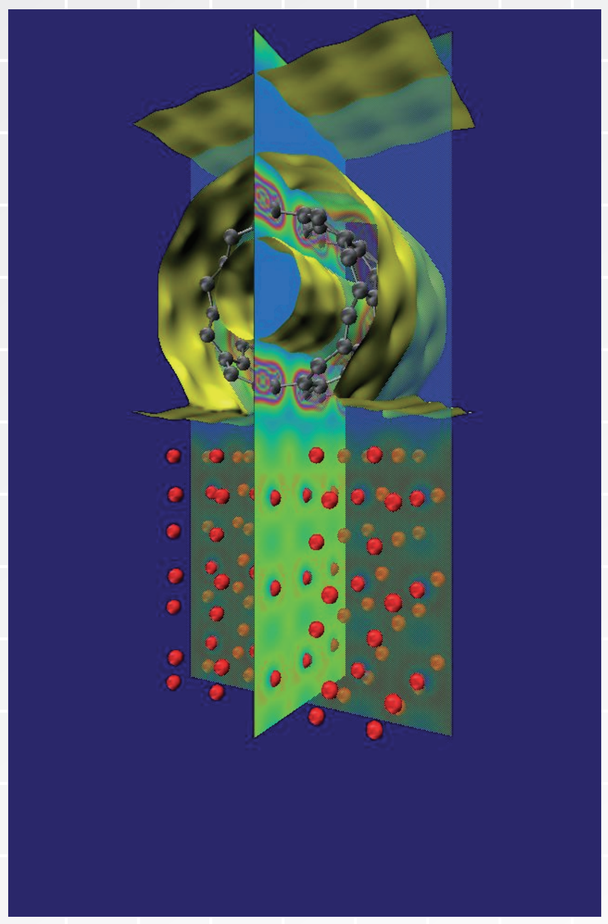
The mechanism of electron hole transfer in a solvated double-helical DNA has been investigated via QM/MM simulations. The results provide a direct evidence of a coherent single step charge transfer and show that a double proton transfer has a fundamental role in triggering the charge hopping along the double stranded DNA



Computational Approach to Interface Physics

Generation of a new concept for Shottoky barrier heights

Shottoky barrier heights are very important interface properties that govern fundamental characteristics of many devices such as transistors, diodes and memories. So far, Shottoky barrier heights are analyzed based on the conventional charge neutrality level (ϕ(CNL)) concept. The conventional ϕ(CNL) concept is constructed based on the following two assumptions. (1) Penetration depth of metal induced gap states (MIGS) is deep enough. (2) Metal density of states (DOS) is almost constant. However, our first principles calculations shows that above two assumptions are not satisfied at neither metal/HfO_2 nor metal/carbon nanotube (CNT) interfaces; MIGS cannot penetrate deep HfO_2 and CNT due to HfO_2 large band gap and geometrical restriction of CNT. Moreover, occupied DOS is much larger than unoccupied DOS in the typical large work function metals such as Au and Pt. This means that the conventional ϕ(CNL) concept can be applicable to neither metal/HfO_2 nor metal/CNT interfaces. .



We have generated a new concept of generalized charge neutrality level (ϕ(GCNL) that is applicable to wide varieties of interfaces based on first principles results. This is because ϕ(GCNL) contains both metal band structures and the atomistic information of interface structures.
Final expression of ϕ(GCNL) is described in eq. (1). Moreover, we have found that the well known "Shottoky limit" can be broken at both metal/HfO_2 and metal/CNT interfaces based on ϕ(GCNL).

$$\phi(GCNL) = E_{VB} + \left(E_g D_{unocc} D_{VB} |t_{m-VB}|^2\right) / \left(D_{unocc} D_{VB} |t_{m-VB}|^2 + D_{occ} D_{CB} |t_{m-CB}|^2\right) \quad (1)$$