DFT Studies of One-Dimensional Systems of Metal-porphyrin Tapes and CuCN Nanowires

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Based on the calculation using the density functional theory, we have investigated the electronic structures of one-dimensional (1D) metal-porphyrin tapes (M-PPT), where M is a metal atom in 3d series.[1] Depending upon the kind of M atom, we first find that M-PPT exhibits varierty of electric properties from a semiconductor to a metal, and even to a half-metal. The band gap is either direct or indirect depending upon the system. Second, our calculation of the quantum transport properties indicate that the bilayer formation of armchair graphene nanoribbons (GNRs) with Zn-PPT or Ru-PPT shows that the bilayer exhibits different conducting properties depending upon the method of inter-unit linkage.[2,3] Third, a ladder type double-stranded 1D system of Zn-PPT bridged by a bypyridyl group (BPY), which was recently synthesized[4], is shown to exhibit a giant Stark effect under the transverse electric field.[5] The effect is as large as that in the boron nitride nanotubes (BNNTs). Fourth, we have also investigated the electronic and magnetic properties of 1D systems of the BPY with M (= Li, V, or Ti) atoms.[6] We find that the difference in the magnetic properties can be understood in terms of different strength of M-M interaction. Finally, hexagonal AuCN or CuCN crytals and their nanowires are shown to have a very high Li storage capacity. Surprisingly, we observe no appreciable volume change after Li is intercalated among three AuCN or CuCN chains with the stoichiometry of AuCN-Li or CuCN-Li. [7]

References

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Figure 1. Electric properties of a bilayer of armchair GNR with triply-linked (TL) and doubly-linked (DL) Zn-PPTs.

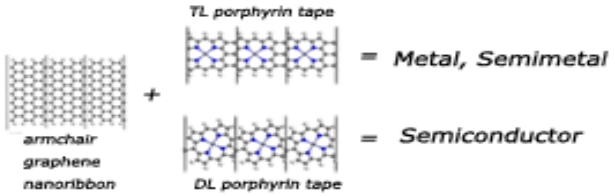

Figure 2. (Left) The geometrical structure of a ladder type double-stranded 1D system of Zn-PPT bridged by a BPY group. (Right) The change of the band gap as a function of the transverse electric field showing the giant Stark effect.

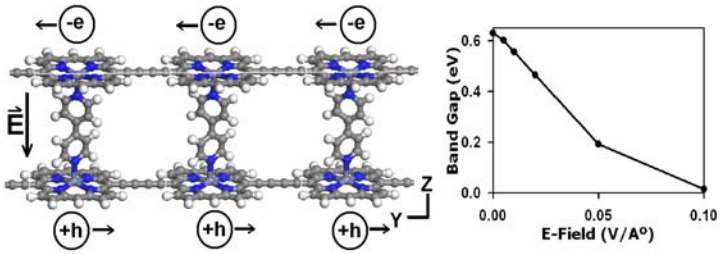

Figure 3. The geometrical structure of $(CuCN)_7$ nanowire which includes 3 Li atoms per primitive cell, showing that Li atoms are located near C≡N group of three adjacent CuCN chains. For clarity, two primitive cells are shown along the *c* axis.