2006 APS March meeting report

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a: CNTs Phonon related topics: (1) In 2000, Berber san determined the thermal conductivity of carbon nanotubes, obtaining an unusual value of 6600 W/m.K at room temperature. These results was confirmed by experiments from Li Shi (UC, Berkeley). They measured a MWNT with diameter 14 nm and the length of the bridging segment 2.5 μm. But both got different temperature dependence of thermal conductivity. Berber san predicts a decrease of thermal conductivity with temperature after 100K and Li Shi observed an increase to get a peak at room temperature. The dependence of thermoelectric power P on the length of length L at 2 different cases (freestanding and substrate supported CNT) was also mentioned, the different relation (P∝1/L and P∝L for freestanding and substrate supported, respectively) between P and L was understood using a diffusive thermal transport model. (2) In CNTs, electron-phonon coupling (EPC) limits the ballistic behavior, the reliable determination of electron scattering length by optical phonons is essential to understand what’s the limit of ballistic transport and is of great scientific and technologic importance in CNTs. Andrea C. Ferrari (Cambridge University) showed that it can be directly determined from the experimental phonon dispersion (Kohn Anomalies) or the Raman D-peak dispersion. They got a simple scaling [ l_{op}=65d/(2n+1) ] between scattering length l_{op} and diameter d and phonon occupations n, by which they may quantify the hot phonon generation. (3) Weak localization in carbon nanotubes has been the subject of intense research. However, Stephan Roche (France) studied the quantum dephasing and decoherence in CNTs by introducing static Anderson-type random potential and dynamical long-range perturbation (phonon), and found that the phonon-induced delocalization effect in the strong static potential.

b: CNTs exciton related topics: Optical spectroscopy transition results were attributed either to optical transition between Van Hove singularities of the valence and conduction bands of 1D system according to the one-electron scheme, or to excitonic transitions according to calculations including multiple interactions. In order to dispel the existing inconsistencies, several experimental results were presented in APS March meeting. (1) Using femtosecond transient absorption technique, Ying-Zhong Ma (UC Berkeley) claimed that they could identify exciton-exciton annihilation and that their observations provide experimental evidence for the excitonic nature. (2) Using two-photon excitation spectroscopy other than conventional linear one-photon absorption and fluorescence spectroscopy, both of which obey different transitional selection rule, Feng Wang (Columbia University, Tony Heinz’s group) demonstrates an excitonic picture which has binding energies 0.4 eV for semiconducting SWNTs. (3) Applying high local electric fields to the partially suspended CNT field-effect transistor (SiO₂, Pd source/drain contacts and a Silicon back gate bearing a trench) under unipolar transport conditions, Jia Chen (IBM) produced high density of excitons and bright infrared emission. Her calculations indicates that the formation of E₂₂ excitons is primarily caused by the annihilation of 2 E₁₁ excitons.

c: Mechanical controlled break junctions (MCBJ) For studying the electronic transport through individual molecules, several experimental techniques like STM, AFM or microfabricated electrodes are available. However, their outputs are largely tailored by the substrates and the distance is usually unaltered. (1) Heiko B. Weber (University of Erlangen) talked about the Mechanically Controllable Break Junctions (MCBJ), its refinement, and the drawbacks as well. The asymmetric conductance (rectification ratio) was observed with numbers of molecules (ex. 1,4-benzenedithiol) in between 2 gold electrodes. If number is bigger than 2, asymmetric effect is switched off; if smaller, effect on. It may realize a fabrication of diode transistor. But he himself said it’s almost impossible to characterize how many molecules between indeed. Also as he said, MCBJ can be improved by appropriate setup like low temperature reducing phonon amplitude, the modification of molecular structure and combining statistical approach (science, 201, 1221). (2) Hydrogen clamp was studied by Sz. Csonka (Hungary) using MCBJ method. [published in PRB 73, 075405 (2006)] A hydrogen molecules incorporated in the gold nano-contact is strong enough to pull a chain of gold atoms, which was suggested by an experimental observation of a well-defined periodic behavior with positive slope in the low-conductance region.

d: Luttinger Liquid and quantum transport (1)The Fermi liquid theory has been quite successful in explaining the electronic transport properties in the higher dimensions due to the weak coulomb interaction. However, some people claimed that even weak coulomb interaction becomes more important in one-dimensional system like CNT, MoSI nanowires and so on. Thereafter we need Luttinger liquid theory to rethink what happens in the 1 dimensional systems. (2) Bernd Rosenow (Harvard University) studied variable range hopping conductivity in 1D disordered electron system and made a few predictions of dc conductivity which seems to be verified by recent experiments on CNTs.
**e: Double exchange or super exchange happens in MoSI nanowires magnetic system?**

(1) Double exchange was used to explain an empirical correlation between the ferromagnetism and electrical conduction observed in La_{1-x}Ca_{x}MnO_3. In that system, Mn^{3+} ion, which is separated with Mn^{4+} by an O^{2−} ion, exchanges d electron with Mn^{4+} through O^{2−}. In our MoSI system, it’s semi-conducting, and does not have conduction d electron for exchange, therefore double exchange may not play a role in magnetism. (2) While super exchange may happen between adjacent Mo_6 octahedra connected by S and induce ferromagnetism! Basically, super exchange was introduced to interpret the anti-ferromagnetism in MnO system. The physical picture is as following: Mn^{2+} - O^{2−} - Mn^{2+} is a ground state for MnO system. Assuming a small perturbation excites the system and may turn it into Mn^{+} - O^{−} - Mn^{2+}, the oxygen ion’s p electrons enters left-handed Mn^{2+} d orbital and this p electron has to carry opposite spin (ex. spin down) since Mn^{2+} has 5 parallel spins (spin up) in its half filled d orbital. Then the spin-up p electron left in the oxygen ion will directly exchange with right-handed Mn^{2+} (all spin down) to get total energy lowered (usually J < 0, spin singlet). Briefly, in the excited state, Mn^{+} correlated Mn^{2+} on the other side by the intermediate O^{−} ion to obtain an anti-ferromagnetism in the new ground state. In our MoSI system, it’s slightly different! Mo (5S^1 4d^5) atom will lose d electron and its d orbital will be less than half filled. In the perturbation process from Mo^{+} - S^{2−} - Mo^{+} to Mo - S^{−} - Mo^{+}, (Mo may be more than +1 charged,) the left-handed exchange happens only if 4d electrons in Mo^{+} and 3p electron from S^{2−} share the same spin direction (Mo^{+} 4d is less than half-filled and Hund’s rule requires biggest S for ground state.). The right-handed exchange is the same as MnO system described above. Thus, Mo on the left hand side correlates with Mo^{+} on the other side by the intermediate S^{−} ion to obtain a ferromagnetism in the new ground state.

**f: people I talked with and exchanged contact information with:** (sorted by the date order)

Taheri@ccs.nrl.navy.mil: Taheri is STM, AFM experimentalist. I talked with her about the plausibility to test MoSI flexibility and magnetism with her STM–AFM combination. Fengwang76@berkeley.edu: Feng Wang is graduated Ph.D. from Tony Heinz’s group. He’s a two-photon excitation and Raleigh scattering spectroscopist. I talked with him about spectrum shift from single to bundle nanotube ropes. 1d MoSI system is an interacting electron system and may have exciton picture in, hopefully we may have some cooperation in the future. phchan@ust.hk: Cho-Ting Chan is a professor from Hong Kong university of science and technology. laiyun@ust.hk: Yun Lai studies photonic crystal calculations in Hong Kong and I talked a lot about MoSI results with him. chenzq@nju.edu: Z-Q Chen is studying La_{0.9}MnO_3 system. I discussed with him about double and super exchange mechanism. And more, mhchen@ufl.edu: M-H chen (optical experimentalist), gsm@mgm.mit.edu: Georgii (CNT experimentalist), phsysw@ust.hk: Ying Wu (photonic theorist).