Final report for IEF project NANOTRAN

Project NANOTRAN was a Marie Curie Intra-European Fellowship centered around nanophysics research conducted between 01/09/2008 and 31/08/2010 at the Physics Department of Lancaster University[1], Lancaster, UK. The Fellow of the project moved from the Research Institute of Solid State Physics and Optics in Budapest to Lancaster University, establishing good collaboration between the two institutions. The project focused on the theoretical study of the electronic properties of nanoscale materials such as carbon nanotubes and graphene nanoribbons, materials which are of importance in molecular electronics. The objectives of the project were two-fold. The primary research objective (**I.**) was to study various carbon-based sub-10-nm systems aimed at understanding how these structures can be utilized in molecular electronics and how they can be improved through functionalization. This included studies of molecular wires sandwiched between metallic or semiconducting leads (**I.1**), encapsulated (filled) single-walled carbon nanotubes (**I.2**), double-walled carbon nanotubes (**I.3**), and graphene strips (**I.4**). The secondary objective (**II.**) of the project was more focused on the development of techniques required to describe the aforementioned structures, including fine-tuning the description of inter-molecular interactions (**II.1**) and looking at electron-phonon coupling (**II.2**). The results of the project should be of importance to researchers in the field of molecular electronics as well as engineers interested in the practical realization of nanoscale electronic devices. The most important achievements of the project are the following.

1. Study of quantum pumping with carbon nanotubes: Nanoscale energy harvesting is now recognized as a possible solution to the problem of powering nanoscale autonomous devices such as NEMS. One possibility is the use of nanomechanical quantum pumps, devices which convert ambient mechanical energy into electrical energy. Project NANOTRAN examined such devices composed of double-walled carbon nanotubes, in which the inner shell is fixed and charge pumping is achieved by rotating the outer shell around it. The results of the research have shown that pumping is surprisingly efficient and that a 1 square micron sized array of such pumps could produce a current of up to 1 microamp, which is more than sufficient to run NEMS devices. Furthermore, the research has shown that the pumping effect is resilient towards disorder, such that the inevitable presence of impurities and lattice defects does not cripple the device at all. It is expected that these results will generate significant interest in the experimental molecular electronics community and motivate engineers to construct quantum pumps based on carbon nanotubes. Related objectives: **I.3** and **II.1**. Publications: pss(b) 246, 2650 (2009); ACS Nano, accepted for publication, DOI: not yet available (2010).

2. Study of functionalized graphene: Recent advances in graphene physics have pointed out that the presence of a single adsorbed molecule can be detected on a graphene ribbon by measuring the conductance, which is a simple and powerful sensing method. While it is not a discriminative method, proper functionalization of a graphene sheet may allow for the identification of the detected molecule, paving the way for single molecule sensing of analyte molecules. This is important in e.g. next generation health care where the reliable detection of small concentrations of toxic molecules can be vital. Project NANOTRAN performed a detailed study of the strength of binding between graphene and various concentrations of adsorbed transition metal atoms as the first step towards designing a discriminating single molecule sensor. This study is not only relevant to single molecule sensing, but also to recent advances in few-atom mass detection. Related objective: **I.4**. Publications: pss(b), accepted for publication, DOI: 10.1002/pssb.201000168 (2010); J. Phys. Chem. C, accepted for publication, DOI: 10.1021/jp107669b (2010).

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3. Study of C_{60} peapods: Fullerene-nanotube peapods (carbon nanotubes filled with fullerene molecules) are materials of great application potential in e.g. spintronics. The Fellow of project NANOTRAN in collaboration with experimentalists studied the Raman spectrum of C_{60} fullerenes encapsulated inside a host single walled carbon nanotube in an electrically charged environment. The aim of the research was to explain unusual features seen in the Raman spectrum during electrochemistry measurements. The research found that the experimental observations are consistent with the view of a small charge penetrating the host wall and occupying the fullerenes. These results help to better understand the nature of the interaction between the host nanotube and the fullerenes, which is essential for countless possible applications of nanotube peapods in general. Related objective: **I.2**. Publications: J. Phys. Chem. C 114, 2505, (2010).

4. Calculating a database of the surface stress of the close-packed surfaces of 5d transition metals: Transition metals are very often used as leads in transport measurements, hence their surface properties are important for e.g. the study of transport through molecular wires sandwiched between such leads. The surface stress is a very important surface parameter which is difficult to measure accurately. The database calculated during the project will aid experimentalists and engineers significantly. Related objective: **I.1**. Publications: J. Phys.: Condens. Matter 21, 095007 (2009).

5. Theoretical study of electron-phonon coupling in graphene: Raman spectroscopy is one of the most useful tools in studying carbon-based materials such as graphene. This research topic focused on calculating the two-phonon LO mode contribution to the Raman spectrum. The calculation relies on the electron-phonon coupling at the corner of the Brillouin-zone, which was obtained by state-of-the-art first principles calculations. Related objectives: **I.4** and **II.2**. Publications: to be submitted to Phys. Rev. Lett.

6. Theoretical study of electron transport through straight carbon nanotube junctions: Double-walled carbon nanotubes can be grown out of the aforementioned peapod structures by annealing. The unique growth environment makes it possible for different types of inner carbon nanotubes to grow inside the same host outer shell, which gives rise to the appearance of straight junctions between them. This research has shown that such junctions are stable and should be possible to identify by measuring the conductance of the outer shell. It is expected that these results will inspire extensive experimental studies on peapod-grown double-walled nanotubes. Related objectives: **I.3** and **II.1**. Publications: pss(b) 246, 2671 (2009); Phys. Rev. B, accepted for publication, DOI: not yet available (2010).

7. Theoretical study of the Raman spectrum of double-walled carbon nanotubes: The inner shells of the aforementioned double-walled carbon nanotubes have a significant curvature which can influence their physical properties. Often these curvature effects are neglected, however, Raman measurements have shown that the most prominent two-phonon line of carbon nanotubes behaves anomalously at low Raman laser excitation energies. The Fellow of project NANOTRAN has shown in collaboration with experimentalists that the anomaly can only be explained by curvature, thereby illustrating that curvature effects are quite important and have serious impact on the physical properties of carbon nanotubes. Related objective: **I.3**. Publications: Phys. Rev. B 81, 125434 (2010).

Overall, the results of project NANOTRAN have brought us closer to understanding how carbon-based nanostructures such as nanotubes and graphene strips can be utilized in molecular electronics and how their physical properties could be improved. The research results are expected to motivate further theoretical research in the field, as well as motivate experimental work; in particular it is expected that the results of this project will lead to the construction of quantum pumps based on carbon nanotubes, to experimental work related to functionalized graphene, and to detailed quantum transport studies of double-walled carbon nanotubes.