



Fifth International Symposium on
Computational Challenges and Tools
for Nanotubes

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Book of Abstracts

CCTN09 Organizers:

Wenhui Duan (*Tsinghua University, China*)

Hisashi Nakamura (*Research Org. for Inform. Sci. &
Technology - RIST*)

David Tomanek (*Michigan State University, USA*)

CCTN09 Program:

8:00-8:15

Registration

8:15-8:30

Opening Remarks: From CCTN05 to CCTN08

Keynote lecture:

8:30-9:15 Haiping Fang

A charge-driven molecular water pump

Invited talks:

9:15-

Andres Ayuela

Substitutional Metal Atoms in Graphene:
Vacancy States Versus Metal Bonding

9:50

9:50-

Arkady V.

Simulations of irradiation-induced effects
in carbon nanomaterials

10:25

Krasheninnikov

Tea Break:

10:15-

11:00

Tea Break

Invited talks:

11:00-

11:35

Leonor Chico

Carbon nanoelectronics: unzipping
carbon nanotubes into graphene
nanoribbons

Lunch Break:

11:15-

13:00

Lunch Break

Contributed talks:

13:00-13:12	Giorgio Lanzani	NH ₃ adsorption and dissociation on a nanosized iron cluster
13:12-13:24	Irina V. Lebedeva	First-principles based kinetic modelling of growth of carbon nanotubes
13:24-13:36	Iann C. Gerber	DFT study of the acid attack on carbon nanotube walls
13:36-13:48	Jian-Ming Lu	Molecular Dynamics Simulation on the Dynamical Behavior of the Water Monomer inside a Single-Walled Carbon Nanotube
13:48-14:00	Andrzej Burian	Structural studies of carbon nanohorns by neutron and X-ray diffraction
14:00-14:12	Lukasz Hawelek	Structural studies of N-doped multi-wall carbon nanotubes by high-energy X-ray diffraction

Tea Break:

14:12-15:00	Tea Break
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Contributed talks:

15:00-15:12	Hong Liu	Electrical Properties of the Deformed Carbon Nanotube Field-Effect Transistors
15:12-15:24	Zeila Zanolli	Defective carbon nanotubes: magnetism, spin transport and gas sensing applications
15:24-15:36	Alireza Nojeh	First-principles calculation of the effect of adsorbates on field-emission current from single-walled carbon nanotubes
15:36-15:48	Alister J Page	Zigzag Grows Faster Than Armchair: Comparisons of SWNT Growth From Self-Consistent-Charge Density-Functional Tight-Binding Molecular Dynamics Simulations
15:48-16:00	Lizhao Liu	Mechanical properties and quantum conductance of carbon nanocoils
16:00-	Santos Hernan	Interface states in achiral carbon

16:12

nanotube junctions: rolling up graphene

Posters

16:12-
17:00

Iann C. Gerber

Influence of nitrogen doping on the radial breathing mode in carbon nanotubes

16:30-
17:00

Irina V. Lebedeva

Multi-level modelling of NEMS based on carbon nanostructures

Keynote Lecture

Invited talk - Saturday, June 20

A charge-driven molecular water pump

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Understanding and controlling the transport of water across nanochannels is of great importance for designing novel molecular devices, machines and sensors and has wide applications, including the desalination of seawater. Nano-pumps driven by electric or magnetic fields can transport ions and magnetic quanta, but water is charge-neutral and has no magnetic moment. On the basis of molecular dynamics simulations, we propose a design for a molecular water pump. The design uses a combination of charges positioned adjacent to a carbon nanotube with an appropriate radius, and is inspired by the structure of channels in the cellular membrane that conduct water in and out of the cell (aquaporins). The remarkable pumping ability is attributed to the charge dipole-induced ordering of water confined in the nanochannels where water can be easily driven by external fields in a concerted fashion. These findings may provide possibilities for developing water transport devices that function without osmotic pressure or a hydrostatic pressure gradient.

Invited Talks

Substitutional Metal Atoms in Graphene: Vacancy States Versus Metal Bonding

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Most popular growth methods of carbon nanotubes rely on the use of catalyst based on transition metals (particularly Ni, Co and Fe), which remain substitutionally attached to the graphenic layer even after purification [1]. Experimentally both Au and Pt atoms have also been implanted on purpose and measured using HRTEM techniques [2]. Here, we investigate systematically the metals of the fourth period between Sc and Zn and those of the 11th(IB) group Cu-Au when place substitutionally in graphene. We find than on one hand, the spin-polarization follows a Slater-Pauling-like behaviour according to the occupation. On the other hand the vacancy states becomes crucial for the description of the bonding to graphene of the late transition elements, starting in Co, and of the group 11 metals [3]. We describe also the ferromagnetic and antiferromagnetic coupling for one of them such as Co in the A and B sites of graphene lattice [4]. Additionally we show the results for the coverage of graphene with 4d elements, taking Zr as an example. The implications concerning the energetic barriers for Zr diffusion on graphene are also commented [5]. These barriers add new insight when bringing them into contact with the mobility experiments of metal atoms in nanotubes and graphene [2].

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[4] E. J. G. Santos, D. Sánchez-Portal, and A. Ayuela (submitted).

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Invited talk - Saturday, June 20

Simulations of irradiation-induced effects in carbon nanomaterials

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The irradiation of solids with energetic particles such as electrons or ions is associated with disorder, normally an undesirable phenomenon. However, recent experiments [1] on bombardment of carbon nanostructures with energetic particles demonstrate that irradiation can have beneficial effects and that electron or ion beams may serve as tools to change the morphology and tailor mechanical, electronic and even magnetic properties of nanostructured carbon systems. Irradiation also gives rise to many interesting phenomena such as irradiation-induced pressure build-up inside carbon nanotubes [3] and onions [4] encapsulated with metals.

We systematically study irradiation effects in carbon nanotubes and other forms of nano-structured carbon. By employing various atomistic models ranging from empirical potentials to time-dependent density functional theory we simulate collisions of energetic particles with carbon nanostructures, and calculate the properties of the irradiated systems.

In this presentation, our latest results on the defect-mediated engineering of the electronic structure of carbon nanotubes [4] will be presented. I will also address the interaction of transition metal atoms with pristine and defected graphene sheets [5]. I will discuss the electronic structure of defected graphene sheets with adsorbed transition metal atoms and identify possible avenues for tailoring the electronic and magnetic structure of graphene by irradiation-induced defects and metal atoms. Finally I will touch upon the response to irradiation of mechanically strained carbon nanotubes and some other low-dimensional systems.

[1] For an overview, see A.V Krasheninnikov, F. Banhart, *Nature Materials*, 6 (2007) 723.

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Carbon nanoelectronics: unzipping carbon nanotubes into graphene nanoribbons

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Quite recently, two experimental groups have reported the unzipping of carbon nanotubes into graphene nanoribbons [1,2].

The partial unzipping of a carbon nanotube can be considered as a seamless union of a carbon nanotube and a graphene nanoribbon. We study these carbon nanostructures, which are found to have remarkable transport properties.

We have found that graphene nanoribbons [3,4] behave at certain energy ranges as perfect valley filters for carbon nanotubes, with the maximum possible conductance [5]. Our results show that nanotubes and the corresponding nanoribbons obtained by unzipping act as optimal contacts for each other, being completely transparent at certain energy intervals.

Application of a magnetic field couples ferromagnetically the edges of the ribbon portion, opening new channels and yielding a large magnetoresistance. Thus, a partially unzipped tube is by itself a magnetoresistive device. Our proposal opens a new route for the design of mixed graphene/nanotube devices [5].

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Contributed Presentations

NH₃ adsorption and dissociation on a nanosized iron cluster

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In doped nanotubes either or both boron and nitrogen atoms replace carbon atoms within the structure and are covalently bound. The main target is to control the electrical properties of the nanotubes, with special attention to control the number of layers. The important industrial potential is demonstrated by developing transparent, conductive, flexible nanotube mats. Despite widespread interest, the chemistry on the surface of BNC catalyst transition-metal nanoparticles is largely unknown though it is believed that the precursor molecules chemisorb dissociatively on their surface and there are major uncertainties in the carbon precursor surface decomposition reaction kinetics and the role of certain species which are believed to etch amorphous the nitrogen/carbon deposits from catalyst particles and thus permit surface decomposition reactions to persist for continuous BNC tube's growth [1,2]. We employed spin-polarized periodic density functional theory (DFT) [3] to study the bonding and chemistry of NH₃ and their fragment on a Fe₅₅ icosahedral cluster. We investigate the site preference for NH₃ with J. P. Perdew, K. Burke, and M. Ernzerhof (PBE) functional [3] and our results, which agree with recent experimental studies, suggest that for NH₃, only the interaction perpendicular at the cluster is favorable ($-0.37 \text{ eV} < \text{B.E.}(\text{NH}_3) < +0.05 \text{ eV}$). When the geometry optimization is started with the molecule placed flat on the surface, it's flipping up during the process. Anyway, also the perpendicular adsorption are not favourable when the hydrogen is toward the surface. Stable geometries of N and H on the high symmetry adsorption site of Fe₅₅ have been calculated as well. Both of the atom present similar behaviour: the hollow or top are the only stable sites and from the bridge sites, the adsorbed migrates on the nearest hollow site. For the atomic nitrogen adsorption, FeN and Fe₃N conformation are observed. The most stable adsorption site is the hollow one (Fe₃N): -1.35 eV . The nitrogen on top sites bind to one iron and the interaction is less favourable: $\text{B.E.}(\text{N}) = -0.05 \text{ eV}$.

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First-principles based kinetic modelling of growth of carbon nanotubes

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Depending on the purpose which carbon nanotubes (CNTs) are grown for, the structure of the nanotubes should meet different requirements. To examine the possibility to control the structure of CNTs grown by chemical vapor deposition, we performed a multi-scale modeling of growth and nucleation of CNTs.

The parameters of dissociation of hydrocarbon precursors on the Ni (111) and Ni(113) surfaces and the characteristics of carbon attachment to graphitic structures on the Ni (111) surface were obtained through density functional calculations. Using these data, the detailed calculations of adsorption and desorption kinetics of hydrocarbons on the Ni surface were performed. The graphite nucleation rate was calculated on the basis of the Fokker-Planck equation. The results of these studies were then used in the macroscopic kinetic model, which describes adsorption of carbon onto the catalyst surface, diffusion of carbon through the catalyst particle, nucleation and growth of CNTs. The model was used to predict the possibility of CNT nucleation under different growth conditions.

The model was applied to study the catalytic activity of different metals on the basis of first-principles calculations of energetics of carbon atoms in the bulk and on the surface of the catalyst particles. The high catalytic activity of Fe and Ni metals and low catalytic activity of Au and Mo were explained. The influence of hydrogen and precursors on the growth of CNTs was investigated. Hydrogen was shown to decrease the carbon supply rate as well as the growth rate of CNTs. An explanation of the experimental results [1] on the effect of hydrogen on diameter, length and defectness of CNTs was suggested. Experimental data on the growth of CNTs from acetylene precursor [2] were well reproduced.

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18, 125602 (2007).

DFT study of the acid attack on carbon nanotubes walls

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Recent studies of metallic nanocatalysts supported by carbon nanotubes have shown very encouraging results concerning activity and selectivity in various type of chemical reactions [1].

Before the deposit of metallic nanoparticles, the pretreatment of the nanotube walls by nitric acid appears to play a crucial role for the dispersion of the nanocatalysts, for the adsorption and the diffusion of the reactants [2]. We present here a theoretical study of this oxydation step, which corresponds to a functionalization of the nanotubes by oxygenated groups. We clearly demonstrate that vacancies strongly influence the oxydation of the graphitic surfaces, with stronger adsorption energies for -OH and -COOH groups. We further concentrate, by comparing molecular models and periodic boundary conditions results, on the reactivity of such defects. The early stages of the nitric acid attack will be presented, which correspond to a possible scenario for the disaggregation of the nanotubes, by the formation of carboxylic groups in the nearest-neighbourhood of vacancies.

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Molecular Dynamics Simulation on the Dynamical Behavior of the Water Monomer inside a Single-Walled Carbon Nanotube

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The dynamical behavior of the water monomer inside a single-walled carbon nanotube (SWNT) is investigated by the molecular dynamics simulation method. The water monomer put initially at random into a SWNT is perturbed by the breathing, lengthening, and shortening modes of a SWNT and moves along the z-axial direction. While achieving the steady state, the water monomer remains the optimal geometrical distance, which is the mean value, and stays closer to the wall of a SWNT instead of to keep nearly the z-axial center of a SWNT. For a (5,5) SWNT with 6.8 Å in diameter, the optimal geometrical distance is 2.56 Å; however, for a (10,10) SWNT with 13.57 Å, it is 3.69 Å. In the present study, the dynamical behavior and motion mechanism of the water monomer, which is inside a SWNT, stirred by the thermal noise of a SWNT are studied. Moreover, the scale, chiral, and temperature effects of a SWNT containing the water monomer are also evaluated.

Structural studies of carbon nanohorns by neutron and X-ray diffraction

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The structure of carbon nanohorns produced by laser ablation at room temperature without a metal catalyst [1] has been studied using the neutron and X-ray diffraction techniques and the molecular dynamics (MD) method. The neutron diffraction measurements were carried out on the GEM (GEneral Materials diffractometer) at the Rutherford Appleton Laboratory. The scattering data were measured up to the scattering vector $Q_{\max}=30 \text{ \AA}^{-1}$ ($Q=4\pi\sin\theta/\lambda$, where 2θ is the scattering angle and λ is the wavelength). The X-ray diffraction data were recorded using a laboratory diffractometer with the monochromatized Ag radiation up to $Q_{\max}=22 \text{ \AA}^{-1}$. The collected diffraction data have been converted to a real space representation in the form of the pair correlation function via the Fourier transform. The structural model consisting of a nanocone with the cone angle approximately 20° and a single-wall carbon nanotube of about 35 nm in length and 2 nm, 2.5 nm and 3 nm in diameter has been computer generated starting from a single graphite layer. The presence of the defects in the form of pentagon-heptagon pairs via the Stone-Wales mechanism has been considered [2]. Then this model has been relaxed using the MD method with the reactive empirical bond order potential [3] for carbon-carbon interaction and the Lennard-Jones potential with parameters for inter-layer interactions [4]. Correctness of a such constructed model has been verified by comparison of the simulations and the experimental data in both real and reciprocal space.

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Structural studies of N-doped multi-wall carbon nanotubes by high-energy X-ray diffraction

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The structure of the nitrogen doped multi-wall carbon nanotubes (~6 at. %) have been studied using the high-energy X-ray diffraction and molecular dynamics (MD) techniques. The diffraction measurements were carried up to a maximum value of the scattering vector $K_{max}=24 \text{ \AA}^{-1}$. The obtained diffraction data were then converted to a real space representation in the form of the pair correlation function. Structural models containing four walled carbon nanotube 300 Å in diameter and 25 Å in length (~35 000 atoms) were computer generated and then relaxed using the Tersoff potential [1] with parameters reported by Matsunaga et al. [2] for carbon-carbon, carbon-nitrogen, nitrogen-nitrogen interactions and the Lennard-Jones potential for inter-layer interactions. According to the previous studies there are three types of nitrogen arrangement in the N-doped carbon nanotubes: in a sp^3 bonding configuration, which represents N atoms in out-of-plane positions, in a sp^2 graphite-like configuration, which represents substitutions of carbon by N atoms, and the pyridine-like N defect (substitutional nitrogen creating a carbon vacancy) [3,4,5]. These three types of nitrogen positions were taken into account. The MD simulations were performed at 2 K. In order to account for the thermal oscillations and static disorder the Debye-Waller factor and the Stone-Wales defects were introduced respectively. For such relaxed models the intensity and pair correlation functions were computed. Correctness of the models was verified by comparison of the simulations with the experimental data both in real and reciprocal space. Effects of three types of nitrogen arrangements (sp^3 bonding configuration, sp^2 graphite-like configuration, and pyridine-like configuration) and the Stone-Wales defects on the resulting structure were investigated.

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Electrical Properties of the Deformed Carbon Nanotube Field-Effect Transistors

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On the basis of the tight-binding theory, we can derive the band structure formula of the deformed carbon nanotube. The results show that the band gap varies with increasing the deformed strength, which points out that the deformation can change the nature of the conductivity of carbon between the metal-type and semiconductor-type. Especially for zigzag nanotubes, there are three different types rules of this translation, which is dependent on the remainder of n divide 3. Furthermore, by using Natori theory on the field-effect transistor we study the current-voltage characteristics of deformed carbon nanotube field-effect transistors. For strain deformation, the conductivity of zigzag nanotube presents different characteristics with the remainder of n and 3. For armchair nanotubes, the conductivity does not change with the strain parameter. However, for torsion deformation, the conductivity rapidly increases, specially for the armchair tube. It has many obviously different conductivity behaviors between zigzag tubes and armchair tubes. At some special torsion angles, the conductivity of zigzag tube and armchair tube has obviously changes, which show that this is the translation between the metal-type and semiconductor-type.

Defective carbon nanotubes: magnetism, spin transport and gas sensing applications

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Carbon nanotubes (CNTs) are renowned in the scientific community for being both a playground for studying fundamental physical properties and for applications in, to mention a few, electronic, spintronic and gas sensing technologies. However, despite the progresses in growth techniques, CNTs always exhibit structural defects [1] and their electronic and transport properties will be affected accordingly [2]. In addition, the presence of defects in carbon-based nanostructures has been seen as source of magnetism [3]. Hence, mastering the physics underlying defected CNTs is crucial not only to model realistic systems but also to design new devices.

The spin-polarized electron transport properties of carbon nanotubes with vacancies are investigated using first principles and non-equilibrium Greens function techniques [4]. Carbon atoms with unsaturated bonds are found to behave as quasi-localized magnetic impurities, coupled by long range interactions. The magnetism of carbon nanotubes with reconstructed mono- and tri-vacancies results in spin dependent conductances and, hence, can be exploited in spintronic devices such as nano-spin valves.

Clarified the properties of CNTs with vacancies, the sensing ability of defected CNTs towards several molecules (NO_2 , NH_3 , CO , CO_2 , H_2O) has also been investigated *ab initio*. Since the adsorption/desorption of molecules induces modulations on the electrical conductivity of the tube, quantum conductances of the CNT-based sensors are predicted, finding that defective nanotubes are sensitive to NO_2 , NH_3 , CO , and H_2O while molecular selectivity is provided by the nature of the charge transfer.

This work is supported by the project Nano2Hybrids (EC-STREP-033311).

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First-principles calculation of the effect of adsorbates on field-emission current from single-walled carbon nanotubes

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Although nanotube-based electron emitters have been investigated for over a decade, there are still many unknowns regarding their emission behavior. For example, it has been debated whether they follow the Fowler-Nordheim model. In some cases the observed current saturation has been attributed to the effect of adsorbates on the emitter tip.

The difficulty has been that first-principles modeling of nanotube emitters under realistic experimental scenarios is computationally very expensive. In particular, although many interesting works have been done on the first-principles investigation of the electronic structure of nanotube emitters, much less has been done on transport simulation in these devices and the calculation of emission current. Moreover, most commercial transport solvers for nanoscale devices focus on devices connected between two electrodes and are not capable of treating vacuum (which is part of the structure in the case of an electron emitter) since they use atomic basis sets that do not extend into vacuum.

We present a calculation of the emission current using our newly-developed three-dimensional, real-space transport solver. The advantage of working in the real space is that vacuum can be defined easily. The electronic structure of the nanotube under an applied field is first obtained using a commercial first-principles package (Gaussian 03 [1]) and the obtained Hamiltonian mapped to the real space to form part of the overall device Hamiltonian (which also includes the vacuum section). The current is obtained using a non-equilibrium Greens function method. It is observed that at high fields the current saturates and the current-voltage characteristics indeed do not follow a Fowler-Nordheim trend, even for a pure nanotube with no adsorbates on the tip. Nevertheless, in many real experimental conditions, due to poor vacuum and existence of residual hydrocarbons or other species, adsorbates could play an important role. In particular, hydrogen is one of the most difficult species to remove even at ultra-high vacuum conditions. Here, we explore the emission characteristics of single-walled carbon nanotubes under various coverage levels of hydrogen, nitrogen and some hydrocarbon molecules. It is observed, for example, that covering the surface of the tip with one monolayer

of hydrogen leads to higher turn-on voltages, but significantly raises the highest occupied molecular orbitals and generally increases the emission current by up to about an order of magnitude in the pseudo-exponential part of the current-voltage characteristics.

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Zigzag Grows Faster Than Armchair: Comparisons of SWNT Growth From Self-Consistent-Charge Density-Functional Tight-Binding Molecular Dynamics Simulations

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The growth of single-walled carbon nanotubes (SWNTs) from Fe₃₈ clusters has been simulated using the self-consistent-charge density-functional tight-binding (SCC-DFTB) method, in conjunction with non-equilibrium molecular dynamics. Growth of the nanotube sidewall was induced by the supply of gas-phase atomic carbon at two different rates to randomly chosen sites in the Fe-C boundary region of both (5,5)-SWNT-Fe₃₈ and (8,0)-SWNT-Fe₃₈.^{1,2} The dependence of SWNT growth dynamics on both the chiral angle of the SWNT (θ) and the rate of carbon supply were therefore elucidated. SWNTs grown in this manner exhibited a large number of defects. In addition, SWNT healing was driven by the relative rates of defect removal and addition in the nanotube sidewall near the SWNT-Fe₃₈ boundary.³ The mechanisms by which adatom, vacancy and 5-7-5 type defects were removed from the SWNT generally took place over timescales of 1-25 ps. These mechanisms were therefore enhanced using lower rates of carbon supply. Using a rapid supply of carbon, an inverse relationship between θ and the SWNT growth rate was established during the early stages of growth. In particular, (8,0)-SWNTs exhibited a mean growth rate *ca.* 20-30% greater than that of (5,5)-SWNTs during the first 40 ps of growth. A recently proposed 'steady-state' model of SWNT growth⁴ suggests that the converse is the case when growth is induced by the diffusion of carbon over the catalyst surface to the SWNT-catalyst boundary. However, average SWNT growth and ring-addition rates of (5,5)- and (8,0)-SWNTs can be explained in terms of the direction in which incident carbon extends the *sp*²-hybridized network with respect to the SWNT axis. It is concluded therefore that the energetic and kinetic properties of SWNT growth mechanisms, and therefore SWNT growth rates, depend on the manner in which carbon den-

sity is supplied to the nanotube itself (*i.e.* direct addition at the SWNT-catalyst interface, as opposed to addition following diffusion over the catalyst surface). It is also postulated that a dependence of SWNT growth rate on the form of carbon feedstock supplied to the SWNT (*i.e.* C, as opposed to C_n) would be observed.

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Mechanical properties and quantum conductance of carbon nanocoils

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Since the discovery of carbon nanotube (CNT) in 1991, low-dimensional carbon nanostructures have attracted great attention due to their potential applications in nanoscale materials and devices. Carbon nanocoil (CNC) or coiled carbon nanotube is a kind of quasi one dimensional (1D) nanostructure, which is similar to CNT except for its helical structure in the whole. Compared to CNT, much less is known about CNC due to the complex geometry structure and difficulty in producing high-crystalline samples. Early theoretical studies were mainly focused on the atomic structure and stabilities, while the mechanical and transport properties of CNC is largely unclear from the theoretically side. In this work, we employed a recently developed tight-binding (TB) total energy model to investigate the structural, mechanical, and electronic properties of single-walled CNC.

Single-walled carbon nanocoils of hexagonal form were built by curling single-walled carbon nanotubes and periodically introducing pentagons and heptagons on the corners. The equilibrium lattice constant and atomic structures of a series of nanocoils were optimized using TB calculations and their Young's modulus can be obtained. 1D electronic band structures were also computed within the TB model. Comparative density functional calculations on smaller nanocoil show the validity of the TB results. The quantum conductance of the carbon nanocoils under compression or elongation was then calculated using a π -orbital tight-binding model incorporated with the non-equilibrium Green's function theory. The correlation between quantum conductance, atomic structure, and mechanical deformation of the CNCs will be discussed. Our theoretical results suggest that carbon nanocoils could be a promising candidate for future nanoelectronics and NEMS devices.

Interface states in achiral carbon nanotube junctions: rolling up graphene

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The ability to form junctions between different nanotubes is the key to develop future nanoelectronic devices [1]. Recently, new advances in the synthesis of carbon nanotube molecular junctions have been achieved, as for example, the controlled synthesis of several carbon nanotube intramolecular junctions, either by current injection between nanotubes [2] or by temperature changes during growth [3]. These intramolecular junctions, which usually present topological defects arising from the connection between tubes of different chirality, often have interface states. Understanding the physics of CNT intramolecular junctions, for which interface states may dominate transport properties, is therefore of great importance.

In this work we study the origin of interface states in carbon nanotube intramolecular junctions between achiral zigzag and armchair nanotubes. The junction between such tubes consists of a whole ring of pentagon-heptagon topological defects. We are able to explain the number and energies by applying the Born-von Karman boundary condition to an interface between armchair- and zigzag-terminated graphene layers. We show that these interface states, costumarily attributed to the presence of topological defects, are actually related to zigzag edge states, as those of graphene zigzag nanoribbons. Furthermore, we explain the different spatial localization of various interface states, which may extend appreciably into either side of the junction [4]. Our results give an alternative explanation to the unusual decay length measured for interface states of semiconductor nanotube junctions [5,6], and could be further tested by local probe spectroscopies.

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Influence of nitrogen doping on the radial breathing mode in carbon nanotubes

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Using density functional theory and a spring constant model we have calculated the change of the radial breathing frequency as a function of nitrogen substitution and concentration. The calculations show that the stable substitution configurations do not favor the formation of nitrogen-nitrogen bonds at low concentration in zig-zag tubes and that the radial breathing frequency depends strongly on the substitution site in the tube. Considering the local symmetry of the radial breathing mode and zone center optical phonons in graphene, we find the ratio of the two frequencies is determined by the ratio of the carbon-carbon bond length and tube diameter.

Multi-level modelling of NEMS based on carbon nanostructures

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At the present time a variety of nanoelectromechanical systems (NEMS) that employ carbon nanotube walls or graphene layers as movable elements are being developed. The crucial issue for the design of such NEMS is the possibility to predict the system behavior at macroscopic operation times (more than 1 s) depending on the microscopic structure of the whole device and its components. We developed a multi-level approach for studying the operation characteristics of the NEMS based on carbon nanostructures.

In the framework of this approach, the tribological properties of NEMS were investigated depending on the parameters and microscopic structure of the system through molecular dynamics simulations. The results of this study for the gigahertz oscillator based on a double-walled nanotube are presented in [1]. These data were then used to describe the dynamic behavior of the NEMS at long simulation times with the help of a phenomenological model [2]. The phenomenological model was applied to obtain the parameters of the system at which the control over the oscillation is possible with an external force. The model was also used to investigate the effect of thermodynamic fluctuations on the oscillator operation.

Significant thermodynamic fluctuations were revealed in the considered NEMS. Thermodynamic fluctuations were shown to lead to a breakdown of the controlled oscillation. Based on the Fokker-Plank equation for the energy distribution function of the gigahertz oscillator and calculations with the phenomenological model we found dependences of the lifetime of the stationary operation mode on the parameters of the system. It was shown that the stability of the NEMS operation subject to thermodynamic fluctuations can be achieved with increasing the amplitude of the control force and the NEMS size.

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