Materials Science and Nanotechnology

Thu, 2016-07-14 12:57 - Rafael Gutierrez [1] **Website:** http://nano.tu-dresden.de/ [2]

Research Type: Theory
Experiment

Activity Summary

The main research activities are focused on concepts, quantitative methods and experiments for understanding and mastering truly nanoscale quantum phenomena. Nanomechanics, nanoelectronics, and information processing are the key issues of our fundamental investigations aiming at developing non conventional strategies for producing and exploiting new devices and materials with intrinsic nanoscale complexity.

Detailed Expertise

1. Molecule-based Quantum Cellular Automata

Conventional semiconductor-based technologies, scaled down to the nanometer scale, show increased heat dissipation, which compromises further miniaturization. Alternatives have been proposed based on the principle of quantum cellular automata (QCA), which have however been implemented in quantum dots, only. QCA offers an alternative vision to binary computing since no current flow is required to encode binary information, and has been considered one of the most promising post-Moore alternatives. Implementation and miniaturization of QCA at the molecular level offer important advantages, including the perspective of room temperature operation, an essential step for industrial exploitation. However, the small sizes of the building blocks lead also to severe challenges when addressing the single elementary units. We are addressing from the modelling point of view the issue of implementing QCA architectures using complex molecular systems. For this, we apply high-level density-functional based methodologies, combined, whenever necessary, with model-based approaches.

Modelling (Rafael Gutierrez): Density functional based approaches; classical and quantum Molecular Dynamics; Coding of binary states in molecular charge states; Intra-molecular charge transfer; Landau-Zener Hamiltonians

References

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2. El Garah, R. C. Perone, A. Santana Bonilla, S. Haar, M. Campitiello, R. Gutierrez, G. Cuniberti, S. Masiero, A. Ciesielski, P. Samorì, Guanosine-based Hydrogen-bonded Scaffolds: G-ribbons and G-quartets Formed in the Absence of Templating Metal Cation, Chemical

Communications 51, 11677 (2015).

3. M. El Garah, A. Dianat, A. Cadeddu, R. Gutierrez, M. Cecchini, A. Ciesielski, P. J. Stang, G.

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2. Quantum transport in complex networks

Although considerable progress has been achieved over the past two decades in the study of the electrical response at the single or few molecules level, a truly molecular scale electronics will necessarily imply the investigation of the charge transport mechanisms in self-organised networks of e.g. metallic nanoparticles functionalized with active molecules, which may serve as starting point for developing unconventional computing strategies. A series of fundamental problems needs to the targeted, including the selection of appropriate functional interconnects, the mechanical stability of the networks, the electrical response of the system at the local level, and charge transport in large scale networks, among others.

Modelling (Rafael Gutierrez): Density functional based approaches; classical and quantum Molecular Dynamics; Non-equilibrium Green's functions techniques; Quantum transport methodologies; kinetic Monte-Carlo approaches

References

1. D. Nozaki, Lokamani, A. Santana Bonilla, A. Dianat, R. Gutierrez, G. Cuniberti, Switchable switchable negative differential resistance induced by quantum interference effects in porphyrin-based molecular junctions, J. Phys. Chem. Letters 6, 3950 (2015)

2. T. Ghane, D. Nozaki, A. Dianat, R. Gutierrez, S. Yitzchaik, J. Chinta, M. Calame, A. Vladyka, G. Cuniberti, Interplay between Mechanical and Electronic Degrees of Freedom in π-Stacked Molecular Junctions: From Single Molecules to Mesoscopic Nanoparticle Networks, J. Phys. Chem. C 119, 6344 (2015).

3. Planar atomic scale quantum architectures

The group is developing quantum technology based on single molecular and atomic manipulation to create atomic circuits and logic gates. Our aim is to investigate quantum information processing and data transmission in atomic and molecular structures. We are exploring planar atomic and sub-molecular scale electronic devices on passivated semiconducting surfaces with atomic scale precision and reproducibility. We combine scanning tunneling microscopy (STM) and spectroscopy

(STS) at low temperature with atomic and molecular manipulation, including hydrogen extraction from passivated surfaces and on-surface chemical synthesis of molecular devices and wires by coupling of precursors. From the modelling point of view, we are addressing the modelling of the charge transport properties of planar, atomic-scale dangling bond circuits on silicon surfaces. Special focus is devoted to the control of the electrical response of these structures via quantum interference effects, AC-fiels, and functionalization with molecular switches.

Experiment (Francesca Moresco): Low-temperature scanning tunneling microscopy, spectroscopy, and manipulation

Modelling (Rafael Gutierrez): Density functional based approaches; classical and quantum Molecular Dynamics; Non-equilibrium Green's functions techniques; Quantum transport methodologies

References

1. R. Ohmann, C. Toher, J. Meyer, A. Nickel, F. Moresco, G. Cuniberti, Quantum coherence of bulk electrons on metals revealed by scanning tunneling spectroscopy, Phys. Rev. B 89, 205433 (2014)

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