様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９　（共通）

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平成　２９　年　　８　月　１６　日現在

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研究課題名（和文）First-principle device simulation

研究課題名（英文）First-principle device simulation

研究代表者

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交付決定額（研究期間全体）：（直接経費）　　2,100,000円

研究成果の概要（和文）：非平衡グリーン関数（Nonequilibrium green's functions NEGF）によるデバイスの第一原理電気伝導計算．NEGFとorder-N density functional theory（DFT）を組み合わせ、電子とフォノンの輸送を研究しました。 導電性高分子、金属デバイス、ハイブリッドシステムについて研究した。特に私たちはミクロンスケールのチャネル材料とナノ構造システムを目指しています。アプリケーションは高性能な計算（ハイ・パフォーマンス・コンピューティング High performance computing, HPC）に最適化されています。

研究成果の概要（英文）：Nonequilibrium green’s function (NEGF) were combined with order-N first principles calculations to study the electronic and phononic at an atomistic level using large scale simulations. We studied conducting polymers, metallic devices, and hybrid systems. We aim to study materials with channels materials in the micron regime and nano-structured systems. The method has been optimised for high performance computing (HPC).

研究分野：　Physics

キーワード：　Device simulations　DFT　Green's functions　Quantum transport

１．研究開始当初の背景

Atomistic device simulating are becoming an indispensable tool to develop novel materials and devices structures. Using an atomistic first principles approach allows to screen and tailor novel materials.

２．研究の目的

Developing a first principles method for transport simulations in nano structured devices in the micron regime.

３．研究の方法

Here we combined nonequilibriums Green's function techniques with order-N first principles calculations to obtain (i) electron and (ii) phonon transport properties.

４．研究成果

Using large-scale computational simulations we studied:

1) Transport based on an order-N DFT method for large channel devices.

2) Phonon transport using a first principles approach.

3) Comparing our first principles transport calculations with molecular conductance measurements obtained from scanning tunneling break junction experiments.

In the following we outline the subjects sketched above and give the main results:

1. Nonequilibrium Green's function (NEGF) method was combined with the order-N code CONQUEST to perform large scale transport simulations. The method has been applied to highly conducting polymers of length between 50 nm to 100 nm (Fig. 1) which are connected to graphene electrodes. 【 1. (Unpublished)】

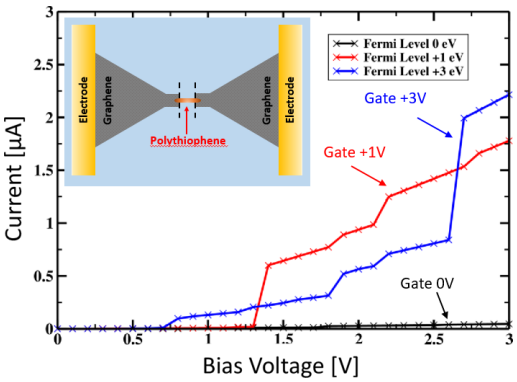

Fig. 1 Calculated current-voltage (I-V) characteristic for different back-gate voltage (polymer length 100 nm)

2. Ballistic phonon transport based on (i) first-principles methods and (ii) classical molecular dynamic simulations were studied for two terminal molecular devices. We could show that the interface properties are largely determine the phonon transport through metal / molecular conductor / metal devices (Fig. 2). Comparing our fully first principles calculations with classical reverse nonequilibrium molecular dynamics simulations of the phonon thermal conductance shows for high temperatures a good agreement between both approaches provided that appropriate force-fields are available. For lower and intermediate temperatures the molecular dynamics approach fails due to missing quantum mechanical effects【2.】

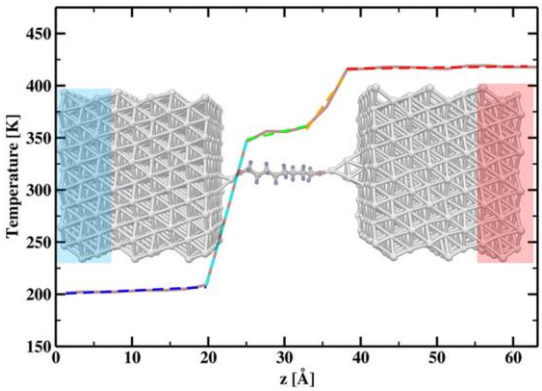

Fig. 2 Temperature profile across the junction【2.】.

3. Using accurate first principle (DFT+∑) based calculations of the conductance we investigated quantum interference in molecular conductors, showing excellent agreement with experiment. We can clearly show that the well-known orbital selection rule can be directly related to quantum interference effects【3.】. Besides the first principles calculations we provide a detailed and rigorous derivation of the orbital selection rule. Our results are demonstrated for tetraphenyl based molecular devices. The calculations allow us to unambiguously assign the experimentally observed conductance information to specific tetraphenyl isomers (Fig. 1).

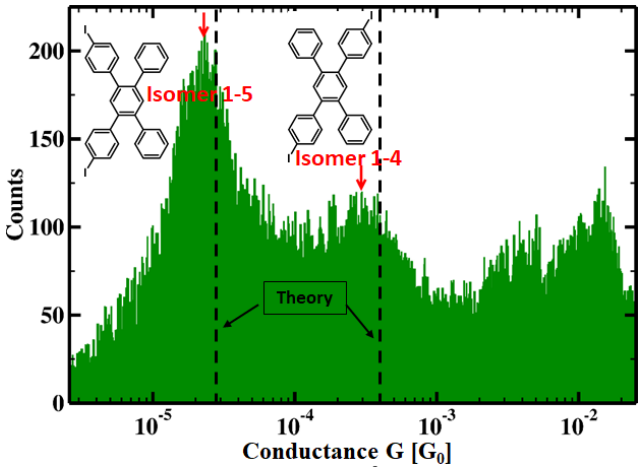

Fig. 3 Measured and calculated molecular conductance for the two considered tetraphenyl isomers.

4. Metallic atomic nanowires made of monovalent (example in Fig. 1) and multivalent metals were studied. Particular attention was paid to the possibility of electrochemically gating the devices. The simulations are compared with conductance measurements in electro chemical environments【4. (Unpublished)】.

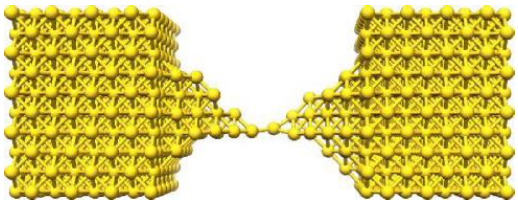

Fig. 4 Example of Gold (monovalent metal) nanowire.

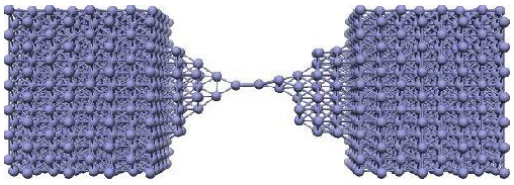

Fig. 5 Example of Zinc (multivalent metal) nanowire.

５．主な発表論文等
（研究代表者、研究分担者及び連携研究者には下線）

〔雑誌論文〕（計　2　件）

[1] Unpublished

[2] M. Buerkle, Y. Asai, **Sci. Rep.**, 7, 41898 (2017)

[3] M. Buerkle, L. Xiang, G. Li, A. Rostamian, T. Hines, S. Guo, G. Zhou, N. Tao, Y. Asai, **J. Am. Chem. Soc.,** 139 (8), 2989 (2017)

[4] Unpublished

６．研究組織

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