行政院國家科學委員會補助專題研究計畫 ■ 成 果 報 告 □期中進度報告

（計畫名稱）

計畫類別：■個別型計畫　□整合型計畫
計畫編號：NSC　97　－　2112　－　M　－　009　　－　001　－　MY3
執行期間：　97　年　8　月　1　日至　100　年　7　月　31　日

執行機構及系所：交通大學電子物理系

計畫主持人：陳煜璋
共同主持人：
計畫參與人員：
博士後: 劉玉申、許程荐
碩士研究生:陳譯仁、姚宣德、曾宜倫、陳彥廷、高毓謙、吳佳翰、黃寶節、翁柏徨、李承智、陳昱璋、許書維、劉韋麟

博士研究生:江吉偉

成果報告類型(依經費核定清單規定繳交)：□精簡報告　■完整報告

英文摘要:

In this 3-year project, we propose to study the transport properties in nano scale junctions. This project can be casted into two categories: spin-unpolarized transport and spin-polarized transport. For spin degenerate case we plan to continue our previous works on the transport properties in nano scale junctions. We will investigate the properties of electron transport in atomic/molecular bimetal junction, including the effect of gate field and many-body effects occurred in this system. We will study the fundamental physical phenomena happened in nano junction, such as effects of local heating, inelastic current, shot noise, and current induced force. All these basic research can contribute to understand the fundamental physics in nanojunction and directed towards the design of new form of electronics devices based on atom/molecule system.

In addition, we will extend our research to the transport properties of spin-polarized electrons in nano scale junction. We propose to develop new theories and new codes in the framework of density functional theory to study possible molecular spintronics devices." Molecular spintronics" is a brand new field and we expect that it is the way for us to stay in the frontier researches. We plan to investigate the role of spin electrons played in the molecular junction. For example, we plan to replace the metal eletrodes by ferromagnets and study tunneling magnetoresistans (TMR). Due to the nature of tunneling and small size of this system, spin is easy to preserve and large magnetoresitance can be anticipated. As a result, molecular system may be a good candidate for spin field effect transistor (SFET). In the long run, we will devote to probe the possibility of new form of spin electronic devices at atomic/molecule scale based on our researches.

計畫中文摘要:

本研究計畫為三年期的計畫。計畫內容區分為兩部分：第一部分是分子電子學的研究。以我們過去所發展關於分子電子學第一原理計算與多體理論作為研究基礎，繼續探討奈米接面系統的電子傳輸性質，如閘極效應、local heating, shot noise, inelastic current, current induced force 等多體效應，並進一步研究分子電晶體的可行性與機制。第二部分是分子自旋電子學的研究。我們計畫將我們目前分子自旋簡併系統的理論和計算，推廣到分子磁自旋系統的理論和計算。我們計畫將分子系統的金屬電極以磁性金屬電極取代，並且考慮原子的自旋軌道偶合效應。由於此系統的尺度微小，所以電子自旋容易保存，加上電子隧穿特性的影響，此系統的 TMR (tunneling magnetoresistance)效應預期會很顯著，這也是我們投入分子系統的自旋電子輸運理論研究的原因。我們預期此系統是有潛力應用於奈米級磁自旋電子元件的製作，例如 spin field effect transistor(SFET)等自旋電子元件等。我們計畫以密度泛函理論(DFT)計算方式，計算分子電子自旋系統的接面性質，研究電子磁自旋的輸運性質並探討此新穎系統的多體物理現象。我們將探討磁自旋分子元件的物理機制與材料特性，朝著分子磁自旋電子元件設計的方向努力。奈米接面系統的電子磁自旋輸運性質，這是一個非常新穎的研究領域，需要開發新的理論與程式，是非常有趣且具挑戰性的研究工作。

一、前言

首先感謝國科會對本計畫的經費補，本研究計畫是為期三年研究計畫，研究的主題是以第一原理計算方式研究奈米接面(nanojunction)的電子傳輸性質，包括熱電效應、高階量子噪音、電子自旋機制與影響等。我們是以多體理論配合密度泛函理論第一原理計算的方式，研究奈米分子接面的電子與熱電性質。

在本計畫支助下，我們的研究主題與本計畫人力配置如下:

(A) 電聲子交互作用產生的局部熱效應與IETS頻譜:

研究苯環分子接面系統分子震盪與電子交互作用。

參與人員:曾宜倫。

(B) 電流的量子漲落(Shot Noise):

研究鋁原子接面的電流的量子漲落與金原子接面電聲子交互作用對電流的量子漲落的影響。

參與人員:劉玉申、李承智、高毓謙。

(C) 分子動力學模擬奈米接面系統的熱電流(Thermal Current MD Simulation):

參與人員: 吳佳翰、翁柏徨、陳昱璋、許書維、劉韋麟。

(D) 分子接面的熱電性質(Thermoelectricty):

參與人員: 劉玉申、陳譯仁。

(E) 分子接面Peltier Effect 與致冷機 與 熱電發電機(Thermoelectric Cooling effect、Molecular Refrigerator, and Power Generator):

參與人員: 劉玉申、姚宣德。

(F) 分子接面電極部分的模擬研究:

參與人員: 黃寶節、姚宣德。

(G) 分子接面電極部分的模擬研究密度泛函超軟虛位能與CDDFT的基礎研究:

參與人員: 黃寶節、陳彥廷、江吉偉。

二、研究目的

最近十年來，奈米電子元件的研究形成一個新興的領域。隨著科技的的發展，電子元件尺寸以對數函數的速度的縮小。當電子元件縮小，不僅可以節省晶片空間，加快浮點運算速度，更可以使單位晶片容納更多的電子元件，使之具備更複雜的功能，同時也可以減少熱能的產生而節省能源，使得電子元件的運作更為穩定。因此分子電子學已經成為未來電子學的願景，引起許多不同領域的科學家們的共同興趣，相繼投入相關研究。一般預期奈米電子元件將對未來的電子工業將產生革命性的影響。同時也會刺激新的理論模型發展和實驗技術創新。

電子元件的大小在如果微米尺度下，輸運電子的性質可以用自由電子氣體來近似描述，系統的導電特性和物理機制可以用半古典理論方式解釋。但是當電子元件的尺寸縮小至奈米大小時，電子的波動性質和原子分子的特性將顯現，並扮演重要的角色。傳統電子學的理論和半古典模型可能不再適用。研究電子的輸運過程，不可或缺的必須考慮原子分子的特性、電子的 wave nature 和量子效應的因素。這個嶄新的系統引起不同領域科學家們的研究興趣，促使奈米接面系統(nanostructures bridged via source-drain electrodes)電子傳輸性質的相關研究形成一個快速發展而且充滿挑戰的新領域。

在實驗上，製作高品質並且可以重覆量測驗證的奈米分子元件是很大的挑戰。主要的原因之一實驗學家難以掌握如此小尺度下，接面的品質和特性，尤其是 contact 的性質。但是隨著研究人員的不斷的努力，實驗技術已有長足的進步。可被重複量測驗證的系統(eg., alkanethiols, oligophenylene molecular junctions)逐漸地被發展出來。在理論計算方面，各種理論模型也是蓬勃發展當中。

我們的研究是利用密度泛函理論，以第一原理計算的方式，探討奈米接面(nanojunction)的電子傳輸性質，除了 I-V characteristics 的計算以外，我們也研究此系統的其他效應，例如電流的量子漲落、電流引發的原子交互作用力、電聲子交互作用所引起的能量消耗、分子振動對電流和溫度的影響、閘極對 I-V characteristics、熱電效應、電子自旋效應等。我們希望能夠繼續擴展我們的研究領域，進一步幫助奈米接面電子輸運的機制和特性的了解，期待我們的研究可以發現更多新的物理現象，刺激更多的理論發展和實驗設計。奈米元件埋藏許多未知的物理機制和材料性質，不僅深具基礎科學研究的價值，而且也深具實際應用的潛力。

最近兩年中此領域有許多新的進展，例如 2007 年 Berkeley 的 Group 首先在 SCIENCE 上發表分子接面系統的熱電效應，引起相當大的震撼。目前該論文已經被引用 40 餘次，所以我們也花費相當的資源人力和時間投入該系統的研究。

奈米電子元件和熱電元件是一個新系統，其發展可能會對人類的科技和生活將產生革命性的衝擊，我們希望我們的研究除了基礎物理的探討外，也能幫助了解奈米電子元件在實際設計和運作上可能面對的潛在問題，幫助奈米電子元件和熱電元件普及的早日實現。

三、重要結果

在本計畫經費的資助下，我們研究的兩個主要方向是（a）分子電子學的研究:探討以分子接面系統作為電子元件(例如分子電晶體、分子接面的量子噪音與 counting ststistics)；(b) 分子熱電效應的研究:探討以分子接面的熱電基本物理性質與此系統作為熱電元件(致冷機與發電機)的熱電轉換效率。

重要的結果簡錄如下:

(a) 分子電子學方面的研究:

1. Alkanethiol-based single-molecule transistors

在烷烴硫化物分子接面系統中，研究閘極電位對電流-電壓特徵曲線關係的影響。研究分子電子學的目的是以分子材料為基礎，研發新型態的電子元件。我們以 Alkanethiol(Cn)分子做為分子接面，過去十年來已經被廣泛的研究。原因是該分子材料容易備製，而且會自組成為單一分子厚度的薄膜，所以適合應用於單一分子接面的電流輸運特性的基礎研究。但是該系統的 HOMO-LUMO 能量間隙很大，而且費米能極介於 HOMO-LUMO 能量間隙中間，所以該系統呈現絕緣體的電流特性。電流電壓關係曲線是線性的(見左圖之圖中圖)，電導率也無法有效地被閘極電壓調控，該系統並未呈現有用的電子元件的特性。我們提出將該系統的 H 以 NH2 取代，發現取代後的分子在費米面附近產生新的能態，使的該系統的導電度變大，並產生不對稱的電流電壓關係曲線(見左圖)。我們也發現 NH2 取代後所產生的新能態，可以被閘極電壓有效的調控，使得電導率的大小產生 30 倍以上的變。所以 NH2 取代後的

Butanethiol(C4)具有作為分子場效應電晶體的潛力。

APPLIED PHYSICS LETTERS 93, 222111 (2008)

Alkanethiol-based single-molecule transistors

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(Received 14 August 2008; accepted 16 November 2008; published online 5 December 2008)

We have investigated the transport properties of alkanethiol molecules in the two-terminal and three-terminal junctions by using first-principles approaches. We observe that states around the Fermi levels are introduced in the amino-substituted butanethiol junction. It leads to a sharp increase in the current, which is credited to the resonant tunneling. The current-voltage characteristics suggest that the amino-substituted butanethiol molecular junction may be a promising candidate for field-effect transistors. © *2008 American Institute of Physics*. [DOI: 10.1063/1.3043438]

2. Counting statistics in nanoscale junctions

我們研究量子噪音，在這篇論文中我們首次在有原子結構的接面中，電流的量子自我相關函數。我們計算一至三階 moments of the current，研究 moments of the current 與電子結構之間的關係。

PHYSICAL REVIEW B 83, 035401 (2011)

Counting statistics in nanoscale junctions

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(Received 22 September 2010; revised manuscript received 16 November 2010; published 3 January 2011)

We present first-principles calculations for moments of the current up to the third order in atomic-scale junctions. The quantum correlations of the current are calculated using the current operator in terms of the wave functions obtained self-consistently within the static density-functional theory. We investigate the relationships of the conductance, the second, and the third moment of the current for carbon atom chains of various lengths bridging two metal electrodes in the linear and nonlinear regimes. The conductance, the second-, and the third-order Fano factors exhibit odd-even oscillation with the number of carbon atoms due to the full and half filled π^* orbital near the Fermi levels. The third-order Fano factor and the conductance are positively correlated.

DOI: 10.1103/PhysRevB.83.035401 PACS number(s): 73.63.Rt, 72.10.Bg, 73.21.Hb, 74.40.De

(b) 分子熱電基本物理特性與熱墊軟換機制方面的研究:

我們以密度泛函理論為基礎，研究原子與分子尺度下，電子的量子輸運性質。並進一步研究此系統的量子多體效應。目的是探討分子與原子系統作為新型態的電子元件或熱電元件的可行性。

3. Thermoelectric Efficiency in Nanojunctions: A Comparison between Atomic Junctions and Molecular Junctions

應用第一原理計算，探討單不同長度的原子金屬線與 Alkanethiol(Cn) 的熱電效率(thermoelectric figure of merit ZT)。我們發現一個特徵溫度，當溫度低於特徵溫度時，電子的熱導大於聲子的熱導，ZT 正比於 T 的平方；當溫度高於特徵溫度時，聲子的熱導大於電子的熱導，ZT 趨近一極限值。當長度增長時，原子線的 ZT 增加，但是分子線的 ZT 增反而減少。

Yu-Shen Liu, Yi-Ren Chen and Yu-Chang Chen*

ACS Nano, 3, 3497-3504 (2009).

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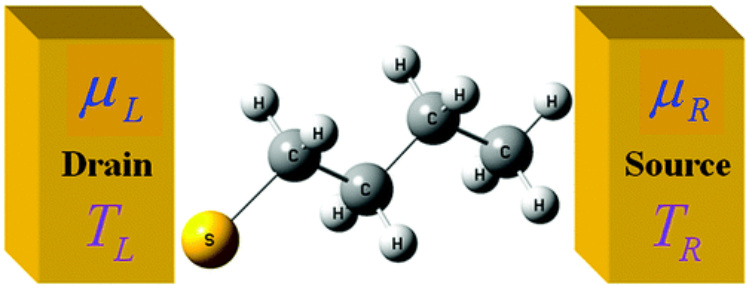
Abstract



Using first-principles approaches, we investigate the thermoelectric efficiency, characterized by the figure of merit ZT, in metallic atomic junctions and insulating molecular junctions. To gain insight into the properties of ZT, an analytical theory is also developed to study the dependence of ZT on lengths (l) and temperatures (T). The theory considers the combined heat current carried by electrons and phonons. We observe a characteristic temperature: $T_0 = (\beta/\gamma(l))^{1/2}$. When $T \ll T_0$, the electronic heat current dominates the combined heat current and ZT $\propto T^2$. When $T \gg T_0$, the phononic heat current dominates the combined heat current and ZT tends to a saturation value. Moreover, the metallic atomic junctions and the insulating molecular junctions have opposite trend for the dependence of ZT on lengths, that is, ZT increases as the length increases for aluminum atomic junctions, while ZT decreases as the length increases for alkanethiol

4. Seebeck coefficient of thermoelectric molecular junctions: First-principles calculations

此篇著作是我們研究分子接面系統熱電效應的開始。以此為基礎，我們即將對分子接面系統的熱電效應展開一系列的理論研究工作，研究此嶄新系統未知的熱電物理性質。深入探討量子現象與原子特性對分子接面熱電效應的影響。目前實驗只能量測到零偏壓下的 Seebeck coefficient，但是我們的理論架構與數值計算，已經能夠進一步延伸，研究該系統的 Seebeck coefficient 如何受到外加閘極電場與外加源漏電壓的影響。可以更深入了解分子接面系統的基本電子結構特性。

PHYSICAL REVIEW B **79**, 193101 (2009)

Seebeck coefficient of thermoelectric molecular junctions: First-principles calculations

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(Received 28 January 2009; published 6 May 2009; corrected 13 May 2009)

A first-principles approach is presented for the thermoelectricity in molecular junctions formed by a single molecule contact. The study investigates the Seebeck coefficient considering the source-drain electrodes with distinct temperatures and chemical potentials in a three-terminal geometry junction. We compare the Seebeck coefficient in the amino-substituted and unsubstituted butanethiol junctions and observe interesting thermoelectric properties in the amino-substituted junction. Due to the novel states around the Fermi levels introduced by the amino substitution, the Seebeck coefficient could be easily modulated by using gate voltages and biases. When the temperature in one of the electrodes is fixed, the Seebeck coefficient varies significantly with the temperature in the other electrode and such dependence could be modulated by varying the gate voltages. As the biases increase, richer features in the Seebeck coefficient are observed, which are closely related to the transmission functions in the vicinity of the left and right Fermi levels.

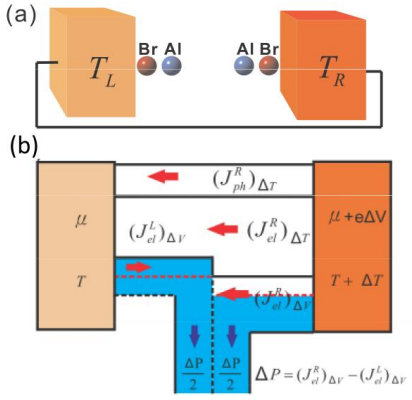
DOI: 10.1103/PhysRevB.79.193101 PACS number(s): 73.50.Lw, 68.43.Pq, 73.40.Jn, 81.07.Nb

5. Atomic-Scale Field-Effect Transistor as a Thermoelectric Power Generator and Self-Powered Device

Yu-Shen Liu, Hsuan-Te Yao, and Yu-Chang Chen*

J. Phys. Chem. C **115**,14988 (2011).

我們以第一原理計算的方式，研究原子尺度的熱電轉換機制。我們提出以 metal-Br-Al-Al-Br-metal 原子接面系統作為原子尺度的熱電發電機。

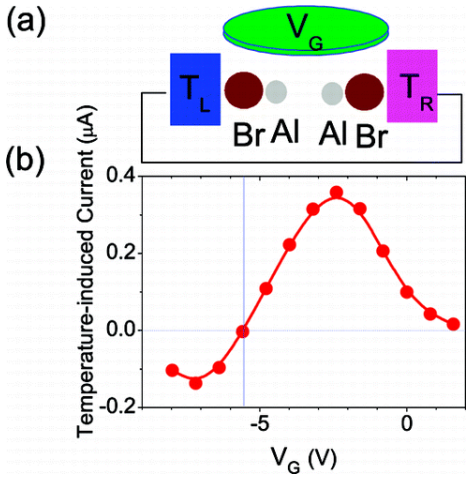


上圖 (a) BrAlAlBr 原子接面系統示意圖。(b) 熱電轉換機制示意圖。

當電極兩端有溫度差時，該系統可以利用熱電效應將由熱端流至冷端的熱流轉換成為的電流。熱能電能的轉換效率，最高可達 9%。當系統外接電池時，其電流與電導的大小可以藉由閘極偏壓加以調控，所以此原子系統本身也是場效應電晶體。在沒有外接電池且形成閉路的狀況下，如果讓電極產生溫度差，原子接面本身仍然可以作為電子元件，而且電子元件本身可以藉由熱能而非電能驅動自己。電流的大小與方向與電導率的大小可以藉由閘極偏壓加以調控。雖然單一原子接面藉由廢

熱所產生的電能只有 10 nW 左右。但是原子接面很小，有機會像 IC chip 一樣，將許多的原子接面以高密度方式集成。在這種情況下，利用廢熱所產生的電能功率將可以非常大。

Abstract



Using first-principles approaches, we have investigated the thermoelectric properties and energy conversion efficiency of the paired metal-Br-Al junction. Owing to the narrow states in the vicinity of the chemical potential, the nanojunction has large Seebeck coefficients such that it can be considered an efficient thermoelectric power generator. We also consider the nanojunction in a three-terminal geometry, where the current, voltage, power, and efficiency can be efficiently modulated by the gate voltages. Such current-voltage characteristics could be useful in the design of nanoscale electronic devices such as a transistor or switch. Notably, the nanojunction as a transistor with a fixed finite temperature difference between electrodes can power itself using the Seebeck effect.

5. Single-molecule refrigerators: Substitution and gate effects

APPLIED PHYSICS LETTERS **98**, 213103 (2011)

Single-molecule refrigerators: Substitution and gate effects

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Using a first-principles approach, we investigate the quantum cooling effects in single-molecule junctions. In comparison with the unsubstituted butanethiol single-molecule junction as a refrigerator, the amino-substituted butanethiol single-molecule junction shows significant enhancement in the coefficient of performance (COP). The enhancement is attributed to the appearance of new states in the neighborhood of chemical potentials due to amino substitution. The COP of butanethiol refrigerator can be improved further by the gate voltages. © *2011 American Institute of Physics*. [doi:10.1063/1.3593379]

6. Effect of Thermoelectric Cooling in Nanoscale Junctions

Yu-Shen Liu, Bailey C. Hsu, and Yu-Chang Chen*

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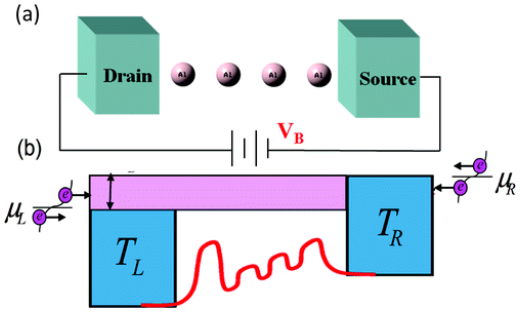
J. Phys. Chem. C, **2011**, *115* (13), pp 6111-6125

我們首先提出以原子接面系統作為制冷機:以原子接面為基礎，利用外加源漏偏壓，以電流帶走熱能，使該原子接面系統具有熱電制冷的效果。因為該系統在電壓小於 20mV 以下時，沒有類似塊材系統焦耳廢熱產生的問題，加上該系統電子以共振隧穿方式傳輸，也避開塊材系統功函數太大的缺點，所以和塊材比較，原子接面系統的制冷效果大幅提升。我們以 4 個鋁原子線為例，以第一原理計算方式，同時考慮了電子輸運與聲子輸運兩者所帶的熱流，探討該系統具有制冷能力的最低工作環境溫度。我們發現原子制冷機在溫度 100K 的低溫環境下，仍然具有熱電制冷能力。和塊材系統(例如真空二極體的必需在 1000K 的高溫下才能有制冷能力)制冷能力相較下，原子制冷機的制冷能力大幅提升。

Abstract



We propose a thermoelectric cooling device based on an atomic-sized junction. Using first-principles approaches, we investigate the working conditions and the coefficient of performance (COP) of an atomic-scale electronic refrigerator where the effects of the phonon's thermal current and local heating are included. It is observed that the functioning of the thermoelectric nanorefrigerator is restricted to a narrow range of driving voltages. Compared with the bulk thermoelectric system with the overwhelmingly irreversible Joule heating, the 4-Al atomic refrigerator has a higher efficiency than a bulk thermoelectric refrigerator with the same thermoelectric figure of merit (*ZT*) due to suppressed local heating via the quasi-ballistic electron transport and small driving voltages. Quantum nature due to the size minimization offered by atomic-level control of properties facilitates electron cooling beyond the expectation of the conventional thermoelectric device theory.

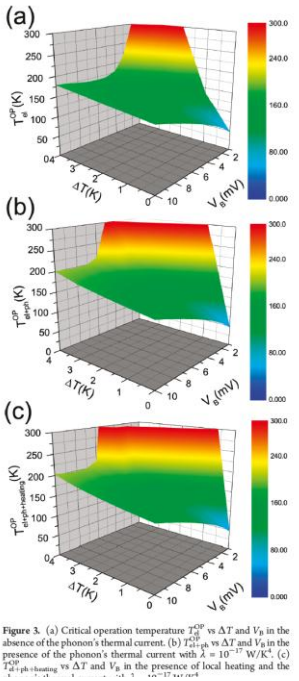


Figure 3. (a) Critical operation temperature T_{ph}^{OP} vs ΔT and V_B in the absence of the phonon's thermal current. (b) T_{el-ph}^{OP} vs ΔT and V_B in the presence of the phonon's thermal current with $\lambda = 10^{-17}$ W/K^4. (c) $T_{el-ph+heating}^{OP}$ vs ΔT and V_B in the presence of local heating and the

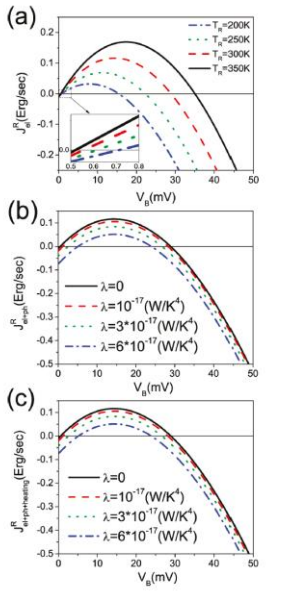


Figure 4. (a) J_{el}^R vs V_B for various values of T_R in the absence of the phonon's thermal current, where $\Delta T = 1$ K. (b) J_{el-ph}^R vs V_B for $\lambda = 0, 1 \times 10^{-17}$, 3×10^{-17}, and 6×10^{-17} W/K^4 in the presence of the phonon's thermal current, where $\Delta T = 1$ K and $T_R = 300$ K. (c) $J_{el-ph+heating}^R$ vs V_B for $\lambda = 0, 1 \times 10^{-17}$, 3×10^{-17}, and 6×10^{-17} W/K^4 in the presence of local heating and the phonon's thermal current, where $\Delta T = 1$ K and

8. Seebeck coefficients in nanoscale junctions: Effects of electron-vibration scattering and local heating

文獻上，我們首度利用密度泛函理論，以第一原理電子結構計算的方式，探討”分子振動”對分子接面之熱電效應的影響。我們發現當 normal mode 的振動方向和電流方向一致時，電聲子交互作用對熱電效應才有顯著的貢獻。當電壓大於 normal mode 的能量時，電子聲子非彈性碰撞造成 Seebeck coefficient 增強的現象。如果進一步考慮電子流經接面所造成的分子侷域溫度升高現象，此侷域溫度將進一步增強分子接面的 Seebeck coefficient。另一方面，當金屬電極溫度升高時，熱擾動會破壞 normal modes 對”Seebeck coefficient-電壓”圖 與 “電流-電壓”圖所產生的微小訊號。

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **83**, 041404(R) (2011)

Seebeck coefficients in nanoscale junctions: Effects of electron-vibration scattering and local heating

Bailey C. Hsu,[1] Yu-Shen Liu,[1,4] Sheng Hsien Lin,[2,3] and Yu-Chang Chen[1,*]

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We report first-principles calculations of inelastic Seebeck coefficients in an aluminum monatomic junction. We compare the elastic and inelastic Seebeck coefficients with and without local heating. In the low-temperature regime, the signature of normal modes in the profiles of the inelastic Seebeck effects is salient. The inelastic Seebeck effects are enhanced by the normal modes and further magnified by local heating. In the high-temperature regime, the inelastic Seebeck effects are weakly suppressed due to the quasiballistic transport.

DOI: 10.1103/PhysRevB.83.041404 PACS number(s): 73.63.Nm, 71.15.Mb, 73.63.Rt

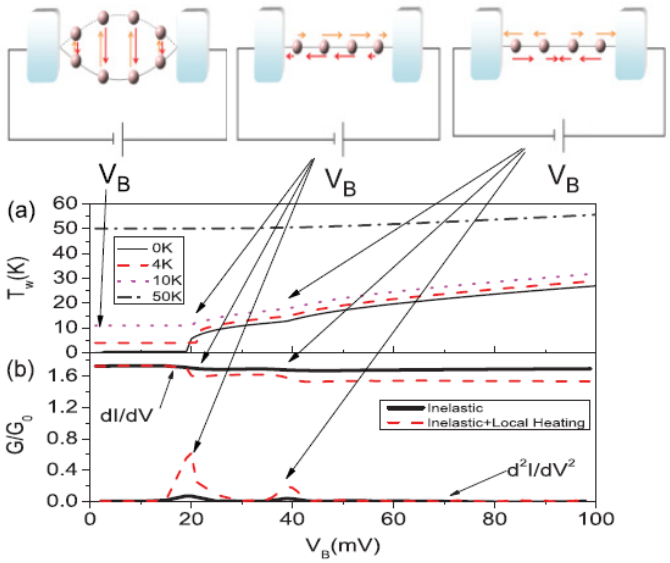

FIG. 2. (Color online) (a) Local temperature T_w as a function of V_B for $T_e = 0$, 4, 10, 50 K. (b) The differential conductance and the absolute value of dG/dV due the electron-vibration interaction without [solid (black) line] and with [dashed (red) line] local heating as a function of bias for $T_e = 12$ K. The schematic shows the normal modes that contribute to the jumps in the local temperature and inelastic current profiles.

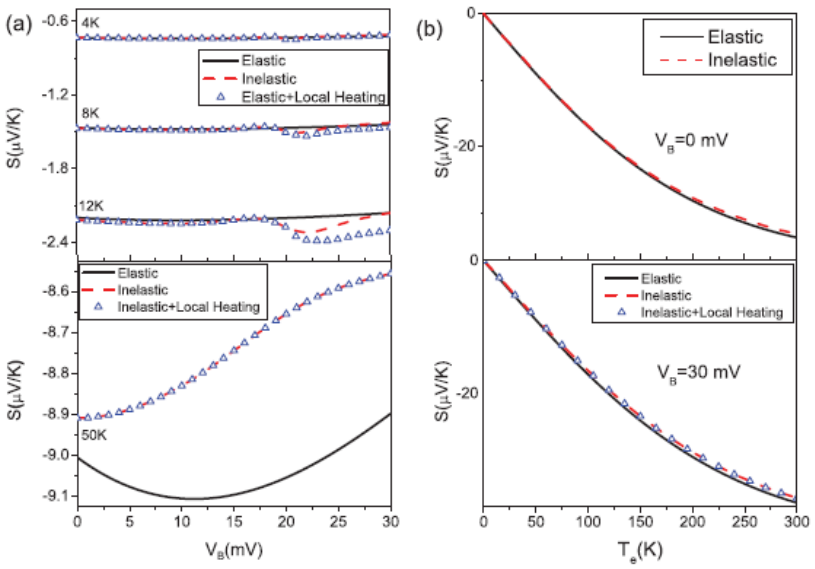

FIG. 3. (Color online) Elastic Seebeck coefficient [solid (black) line], inelastic Seebeck coefficient without local heating [dashed (red) line], and that with local heating [triangle (blue) line] (a) as a function of bias V_B for $T_e = 4$, 8, 12 K (top panel) and $T_e = 50$ K (bottom panel); and (b) as a function of T_e for $V_B = 0$ K (top panel) and and $V_B = 30$ K (bottom panel.)

四、計畫成果自評

在本國會計畫支助下，我們才有能力從事分子電子學的相關研究工作。本研究計畫的計算相當耗費電腦資源，以 Butanethiols 分子系統為例，我們的計算該龐大的分子系統的源漏電壓與閘極電壓與電流的關係。這個計算我們利用了超過 4000 個平面波當基底，利用 250 個 CPU，日夜連續計算了 8 個月才得到較完整的計算結果。我們在此非常感謝國科會過去對本計畫在經費上的支助。我們才有可能建立一個足夠大型的電腦叢集系統，從事如此龐大的計算與研究工作。感謝餐與本研究計畫的博士後與研究生，在大家共同努力下，我們完成了部分的研究工作，也得到了一些具體的研究成果。同時，我們仍然有許多未完成的工作，對這些具挑戰性的問題，我們未來將繼續深入探討。

五、附錄 (本計畫資助所發表之論文)

感謝國科會經費的資助。以下是執行本國科會計畫所發表的期刊論文:

[1] "Seebeck Coefficients in Nanoscale Junctions: Effects of Electron-vibration Scattering and Local Heating."
Phys. Rev. B **83**, 041404(R) (2011).(rapid communication)
Bailey C. Hsu, Y. S. Liu, S. H. Lin, and Y.-C. Chen*

(IF:3.772)

[2] "Counting Statistics in Nanoscale Junctions."
Phys. Rev. B **83**, 035401 (2011).
Y. S. Liu and Y.-C. Chen*
(IF:3.772)

[3] "Effect of Thermoelectric Cooling in Nanoscale Junctions."
J. Phys. Chem. C **115**, 6111 (2011).
Y. S. Liu, Bailey C. Hsu, and Y.-C. Chen*
(IF:4.520)

[4] "Single-molecule Refrigerator: Substitution and Gate Effect."
Appl. Phys. Lett. **98**, 213103 (2011).
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(IF:3.820)

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[6] "First Principle Studyof the Electron Density Distribution in a pair of Bare Metallic Electrodes."
Appl. Phys. A **104**, 325 (2011).
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(IF:1.760)

[7] "Thermoelectric Efficiency in Nanojunctions: A Comparison between Atomic Junctions and Molecular Junctions."
ACS Nano **3**, 3497 (2009).
Y. S. Liu, Y. R. Chen and Y.-C. Chen*
(IF:9.985)

[8] "Seebeck coefficient of thermoelectric molecular junctions: First-principles calculations."
Phys. Rev. B **79**, 193101 (2009).
Y. S. Liu and Y.-C. Chen*
(IF:3.772)

[9] "Alkanethiol-based single-molecule transistors."
Appl. Phys. Lett. **93**, 222111 (2008).
Chun-Lan Ma, Diu Nghiem, and Y-.C. Chen*
(IF:3.820)

本計畫除繳交成果報告外，另須繳交以下出國心得報告：

■赴國外出差或研習心得報告

■赴大陸地區出差或研習心得報告

■出席國際學術會議心得報告

中　華　民　國　100　年　10　月　1　日

國科會補助專題研究計畫成果報告自評表

請就研究內容與原計畫相符程度、達成預期目標情況、研究成果之學術或應用價值（簡要敘述成果所代表之意義、價值、影響或進一步發展之可能性）、是否適合在學術期刊發表或申請專利、主要發現或其他有關價值等，作一綜合評估。

1. 請就研究內容與原計畫相符程度、達成預期目標情況作一綜合評估

■　達成目標

□　未達成目標（請說明，以 100 字為限）

□ 實驗失敗

□ 因故實驗中斷

□ 其他原因

說明：

2. 研究成果在學術期刊發表或申請專利等情形：

論文：■已發表 □未發表之文稿 □撰寫中 □無

專利：□已獲得 □申請中 □無

技轉：□已技轉 □洽談中 □無

其他：(以 100 字為限)

合計發表 9 篇論文表列於 五、附錄 (已發表之論文)

3. 請依學術成就、技術創新、社會影響等方面，評估研究成果之學術或應用價值（簡要敘述成果所代表之意義、價值、影響或進一步發展之可能性）（以500 字為限）

熱電效應的研究是一門很古老的學問，早在 1821 年 Seebeck 就已經發現 Seebeck effect。Seebeck 發現在熱電塊材材料兩端加上不同的溫度，兩端的溫度差異將會使熱電材料兩端產生電位差，此效應可以將熱能轉換成為電能。之後三十年間， Peltier 效應與 Thomson 效應相繼被發現。在 1950 以前，熱電效應的理論發展已經逐漸趨於完備，塊材的巨觀與微觀理論機制解釋已經相當成熟。理論研究顯示 Seebeck coefficient 和材料的電子結構密切相關。

微小結構材料的發展速度非常的迅速，經過三、四十年的發展、微米尺度的微小結構技術已經相當成熟。近年來，微結構材已由微米尺度逐漸進展到奈米尺度甚至觸及原子尺度。應用分子作為電子元件的觀念始於 1974 年 [A. Aviram and M. A. Ratner, Chem. Phys. Lett. 29, 277 (1974)]。直到 1997 年 Yale University 的 Mark Reed 研究團隊，才首次量測到單一分子的電流電壓特徵關係曲線，開啟了分子原子尺度電子元件實際製作與發展的新紀元。

微米尺度下，接面系統的電子輸運性質可以用半古典理論自由電子氣體模型解釋。當微結構縮小至原子與分子尺度，電子的量子效應、波動性質與原子特性更加強烈，半古典電子氣已經無法描述此系統的物理。於是分子原子接面系統的電子輸運性質與物理機制需要新理論模型與解釋。目前世界上已經有的實驗團隊可測量到原子分子接面系統的電導值，同時也有理論團隊致力於研發新的理論架構，以理論方式探討分子接面電子輸運的量子與分子特性。但是分子接面系統的熱電效應，一直到 2007 年才首度由 UC, Berkeley 的 Prof. Majumdar 的實驗團隊率先量測到[Reddy P.; Jang S. Y.; Segalman R. A.; Majumdar A. Science 315, 1568 (2007); Nano Lett. 8, 715(2008); ibid. 9, 1164(2009).]。受到這些實驗的啟發，我們開始分子接面系統熱電效應的研究工作。我們以密度泛函理論為基礎，研究原子與分子尺度下，電子的量子輸運性質。並進一步研究此系統的量子多體效應。目的是探討分子與原子系統作為新型態的電子元件或熱電元件的可行性。我們在理論上首先提出了分子接面系統作為致冷機與熱電發電機的模型，並且理論上研究熱電轉換機制與探討熱電轉換效率。希望藉此開拓新形態的奈米電子元件與奈米熱電元件。

出席國際學術會議心得報告

計畫編號	97-2112-M-009-011-MY3
計畫名稱	奈米接面系統的簡併電子與磁自旋電子的輸運性質(1/3)
出國人員姓名 服務機關及職稱	陳煜璋
會議時間地點	**2009 APS March Meeting** **Monday–Friday, March 16–20, 2009; Pittsburgh, Pennsylvania**
會議名稱	2009 American Physical Society March meeting
發表論文題目	**(1) Abstract: L11.00002 : Electron Transport and Thermoelectricity in Alkanethiol Molecular Junctions** (2) **S1.00128 : Generation of spin polarized current in a semiconductor by an ohmic contact containing ferromagnetic particles**

一、參加會議經過

三月16-20日參加美國物理年會 2009 APS March Meeting: Monday－Friday, March 16－20, 2009; Pittsburgh, Pennsylvania

共計發表一篇口樓報告與一篇壁報論文:

Abstract: L11.00002 : Electron Transport and Thermoelectricity in Alkanethiol Molecular Junctions

3:06 PM–3:18 PM

Authors:

Yu-Chang Chen

(Department of Electrophysics, National Chiao Tung University, Taiwan)

Chun-Lan Ma

(Department of Electrophysics, National Chiao Tung University, Taiwan)

Diu Nghiem

(Department of Electrophysics, National Chiao Tung University, Taiwan)

Yu-Shen Liu

(Department of Electrophysics, National Chiao Tung University, Taiwan)

We investigate the electron transport properties of alkanethiol molecules in the two- and three-terminal junctions by using first-principles approaches. We observe that novel states around the Fermi levels are introduced in the aminosubstituted butanethiol junction. It leads to a sharp increase of the current owing to the resonant tunneling. We also describe a field-theoretic theory combined with first principles approaches to calculate the thermoelectricity. The dependence of the Seebeck coefficient on the biases, gate voltages, and temperatures is systematically investigated Due to the novel states introduced by the amino-substituted butanethiol junction, the Seebeck coefficient could be easily controlled by using gate voltages and biases. When the temperature in one of the electrodes is set to zero, the Seebeck coefficient could vary pronouncedly with the temperature in the other electrode, and such dependence could be enhanced by varying gate voltages.

At finite biases, we also find richer features in the Seebeck coefficient related the density of states in the vicinity of the left and right Fermi levels.

Abstract: S1.00128 : Generation of spin polarized current in a semiconductor by an ohmic contact containing ferromagnetic particles

Authors:

Leonardo Castelano

(Department of Physics, University of California, San Diego)

Yu-Chang Chen

(Department of Electrophysics, National Chiao Tung University)

S.-R. Eric Yang

(Physics Department, Korea University)

Lu Sham

(Department of Physics, University of California, San Diego)

We investigate the possibility of injection of spin polarized current into a semiconductor from an ohmic contact containing ferromagnetic metal (FM) nanodots. The polarization is created by the spin-dependent scattering of the current carriers with the FM dots with aligned magnetizations. The usually inefficient polarization generation due to the resistance mismatch between the metal electrode and the semiconductor is mitigated by the reduction of the mismatch between the FM dots and the heavily doped electrode. When the paramagnetic semiconductor is connected by two such electrodes containing FM dots forming a spin valve system, the magnetoresistance is calculated to be sizable. We report the calculation results for two examples: (i) silicon connected to electrodes of poly-silicon contain the FM dots and (ii) the heavily doped region of InAs as contact.

二、與會心得

會議中聆聽了 BERKELEY PROF. Majumdar GROUP 關於分子系統熱電效應的演講，該 GROUP 是至今唯一能夠量測分子系統熱電效應的實驗團隊。奈米接面系統的熱電效應是一個非常新的研究領域。過去熱電效應的研究局限在塊材系統，分子接面系統的熱電效應直到 2007 年才有第一個實驗數據。目前為止只有三篇實驗 paper，均為 Berkeley University Prof. Majumdar 團隊所量測(分別發表在 2007 Science； 2008 與 2009 Nano Lett.)。該研究成果相當新穎有趣而且具有未來實際應用的潛力。因此我們也投入相當多的人力和時間進行相關的研究。本次會議口頭報告也是受到該實驗的啟發才投入相關的研究。另在會議中也和 Arizona State University 的 PROF. NJ Tao 以及 University of Michigan 的 PROF. Barry D. Dunietzw 討論分子系統熱電相關問題，收穫頗多。

出席國際學術會議心得報告

計畫編號	97-2112-M-009-011-MY3
計畫名稱	奈米接面系統的簡併電子與磁自旋電子的輸運性質(2/3)
出國人員姓名 服務機關及職稱	陳煜璋

會議時間地點	**(1) 2010 APS March Meeting** **Monday–Friday, March 15–19, 2010; Portland, Oregon, USA** (2)The 12th Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN12) Institute of Physics, Chinese Academy of Sciences, Beijing,China on Oct. 26-28, 2009
會議名稱	2010 American Physical Society March meeting
發表論文題目	**(3)** **(i)H14.00004 "Atomic-Scale Thermoelectric Refrigerator"** **(ii)K1.00147 "The Third Order and the Second Order Shot Noise in Nanoscale Junctions from First Principles"** **(2) "Thermoelectricity in atomic and molecular junctions"** **Yu-Chang Chen (Invited talk)**

三、參加會議經過

三月15-19日參加美國物理年會 2010 APS March Meeting: Monday – Friday, March 15 – 19, 2010; Portland, Oregon

共計發表一篇口樓報告與一篇壁報論文:

Session H14: Focus Session: Transport Properties of Nanostructures III: Theory and Computation I

8:00 AM–11:00 AM, Tuesday, March 16, 2010

Room: B113

Sponsoring Unit: DMP

Chair: Jeffrey Neaton, Lawrence Berkeley National Laboratory

Abstract ID: BAPS.2010.MAR.H14.4

H14.00004 : Atomic-Scale Thermoelectric Refrigerator

9:00 AM–9:12 AM

Authors:

Yu-Chang Chen

(Department of Electrophysics, National Chiao Tung University, Taiwan)

Yu-Shen Liu

(Department of Electrophysics, National Chiao Tung University)

We propose a thermoelectric cooling device based on an atomic-sized junction. Using first-principles approaches, we investigate the working conditions and the coefficient of performance (COP) of an atomic junction as an electronic refrigerator. Our research reveals that the absence of local heating and the suppression of the tunneling barrier by the bridging atoms are favorable for the operation of atomistic refrigerators. From the self-consistent DFT calculations, we show that the atomistic refrigerator may operate at temperatures below 100 K. This is a great improvement in comparison with the vacuum diode. We also investigate the impact of the phononic heat current on the capability of refrigeration in the nano-refrigerator. To minimize the adverse effects of the phononic heat current, we suggest creating a poor mechanical link between the nano-structured object and the electrodes while still allowing electrons to tunnel.

Session K1: Poster Session II (2:00 pm - 5:00 pm)

2:00 PM–2:00 PM, Tuesday, March 16, 2010

Room: Exhibit CD

Abstract ID: BAPS.2010.MAR.K1.147

Abstract: K1.00147 : The Third Order and the Second Order Shot Noise in Nanoscale Junctions from First Principles

Authors:

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We propose a field-theoretic theory allied to first principles calculations to study the third order cumulant of quantum shot noise in nanoscale junctions. Our starting point is the second-quantized field operator in terms of the effective single-particle wave-functions obtained self-consistently within the density-functional theory. The approach is valid in both linear and nonlinear response regime and is particularly suitable in studying the third order quantum shot noise in atomic-scale junctions. As an example, we investigate the conductance, the second order shot noise, and the third order shot noises in the carbon atomic wires connected between two metal electrodes. We observe that all these physical quantities display an oscillatory behavior for even and odd number of carbon atoms.

(ASIAN12)

Title: Thermoelectric Properties in Nanojunctions

ABSTRACT

The miniaturization of thermoelectric nanojunctions raises a fundamental question: do the thermoelectric quantities of the bridging materials in nanojunctions remain to display material properties or show junction properties? In order to answer this question, we investigate the Seebeck coefficient *S* and the thermoelectric figure of merit *ZT* especially in relation to the length characteristics of the junctions from the first principles approaches. For *S*, the metallic atomic chains reveal strong length characteristics related to strong hybridization in the electronic structures between the atoms and electrodes, while the insulating molecular wires display strong material properties due to the cancellation of exponential scalings in the DOSs. For *ZT*, the atomic wire remains to show strong junction properties. However, the length chrematistics of the insulation molecular wires depend on a

characteristic temperature $T_0 = \sqrt{\beta/\gamma(l)}$ around 10 K. When $T < T_0$, where the electron transport dominates the thermal current, the molecular junctions remain to show material properties. When $T > T_0$, where the phonon transport dominates the thermal current, the molecular junctions display junction properties.

四、與會心得

會議中遇見 Arizona State University 的 Prof. NJ Tao，談了一些是否將來可以在奈米接面熱電系統的研究合作。在所有的 Talk 中印象最深刻的是凌聽了 G.D. Mahan 關於熱電領域的邀請演講，他對熱電領域的發展，作了一番幽默且有趣的介紹。值得回憶紀錄的是，隔天在我的 oral presentation 前，G.D. Mahan 特地進到我的 Section 聽演講，當我的演講結束後，他就離開了。顯然他特別對我們所提出的原子致冷機具有相當高的興趣。另一場印象深刻的演講是 Steven Louie 關於 Exchange-correlation energy 的 GW 近似，應用到分子電子學 DFT 理論計算的研究。當他演講結束後，特地去找他談是否可以合作 GW calculation 應用到我們的程式計算的機會。

出席國際學術會議心得報告

計畫編號	97-2112-M-009-011-MY3
計畫名稱	奈米接面系統的簡併電子與磁自旋電子的輸運性質(3/3)
出國人員姓名 服務機關及職稱	陳煜璋
會議時間地點	**(1) 2011 APS March Meeting:** **Monday–Friday, March 21–25, 2011; Dallas, TX, USA** **(2) 量子输运理论和纳米电子学模拟国际研讨会** Department of Physics, Remin University of China Aug. 10-18, 2011
會議名稱	2010 American Physical Society March meeting

發表論文題目	**(1) 2011 APS March Meeting** **(i) T24.00002 “Seebeck Coefficients in Nanoscale Junctions: Effects of Electron-Vibration Scattering and Local Heating”** **(ii)K1.00147 “Counting Statistics in Nanoscale Junctions from First Principles”** **(2) 量子輸運理論和納米電子學模擬國際研討會** **(i) “Current Streamline Flow on Current-induced Effects in Highly Asymmetric Molecular Junctions” (30 mins)** **(ii) “Quantum Transport and Thermoelectric Properties of Nanoscale Junctions and their Device Applications” (90 mins)** **Yu-Chang Chen (Invited talk)**

五、參加會議經過

(1) 2011 March Meeting

我和博士後許程荐分別發表一篇口頭報告如下

Session T24: Focus Session: Quantum Transport Simulations and Computational Electronics -- Disorder

2:30 PM–5:06 PM, Wednesday, March 23, 2011

Room: D167

Sponsoring Unit: DCOMP

Chair: Massimo Fischetti, University of Texas at Dallas

Abstract ID: BAPS.2011.MAR.T24.2

Abstract: T24.00002 : Seebeck Coefficients in Nanoscale Junctions: Effects of Electron-Vibration Scattering and Local Heating

3:06 PM–3:18 PM

Preview Abstract

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Yu-Chang Chen

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We report first-principles calculations of inelastic Seebeck coefficients in an aluminum monatomic junction. We compare the elastic and inelastic Seebeck coefficients with and without local heating. In the low temperature regime, the signature of normal modes in the profiles of the inelastic Seebeck effects is salient. The inelastic Seebeck effects are enhanced by the normal modes, and further magnified by local heating. In

the high temperature regime, the inelastic Seebeck effects are weakly suppressed due to the quasi-ballistic transport.

Session T24: Focus Session: Quantum Transport Simulations and Computational Electronics -- Disorder

2:30 PM–5:06 PM, Wednesday, March 23, 2011
Room: D167
Sponsoring Unit: DCOMP
Chair: Massimo Fischetti, University of Texas at Dallas
Abstract ID: BAPS.2011.MAR.T24.5

Abstract: T24.00005 : Counting Statistics in Nanoscale Junctions from First Principles

3:42 PM–3:54 PM

Authors:

Yu-Chang Chen
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We present first-principle calculations for moments of the current up to the third-order atomic-scale junctions. The quantum correlations of the current calculated in terms of wave functions obtained self-consistently within the static density functional theory are also demonstrated herein. Relationships between the conductance, the second, and the third moment of the current for carbon atom chains of various lengths bridging two metal electrodes in the linear and nonlinear regimes are investigated. The conductance, the second-, and the third-order Fano factors exhibit odd-even oscillation with the number of carbon atoms. The third-order Fano factor is positively correlates with conductance.

(2) 量子輸運理論和納米電子學模擬國際研討會(在 2011 年 8 月 10 日至 2011 年 8 月 19 日在中國人民大學召開)

電流密度流線對高度非對稱的分子接面的影響/Current Streamline Flow on Current-induced Effects in Highly Asymmetric Molecular Junctions

Bailey C. Hsu (許程薦), Allen Tseng(曾宜倫), and Yu-Chang Chen* (陳煜璋)

Department of Electrophysics, National Chiao Tung University, Hshinchu 30010, Taiwan

【摘　　要】/Abstract:

Electron transport in a single-molecule molecular junction, where the molecule is sandwiched between two electrodes, has been investigated extensively in the pursuit of extreme device miniaturization. A major concern for single-molecule junctions is the fundamental properties of current-induced effects due to nonequilibrium electron transport at finite biases. These effects are efficient tools to explore the

single-molecule signatures from quantum mechanical perspectives, and thus are important and interesting from theoretical and experimental points of view. From first-principles approaches, we illustrate that the current-induced forces and the selection rule for inelastic effects are highly relevant to the current density in an asymmetric molecular junction. The curved flow of current streamline around the asymmetric molecule may induce a net torque, which tends to rotate the benzene molecule, similar to the way a stream of water rotates a waterwheel. Thus, the Pt/benzene junction offers a practical system in the exploration of the possibility of atomic-scale motors. We also enumerate examples to show that the use of selection rule can lead to misjudgement of the importance of normal modes in the inelastic profiles when the detailed information about the current density is not considered.

【參考文獻】/ References:

[1] Bailey C. Hsu, Allen Tseng, and Y.-C. Chen*, arXiv:1106.1701.

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[3] M. Di Ventra, Y. C. Chen, and T. N. Todorov, Phys. Rev. Lett. **92**, 176803 (2004).

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奈米接面的電子傳輸性質與熱電性質與其原件上的應用/**Quantum Transport and Thermoelectric Properties of Nanoscale Junctions and their Device Applications**

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Department of Electrophysics, National Chiao Tung University, Hshinchu 30010, Taiwan

【摘　　要】/Abstract:

Density-functional theory (DFT) combined with Lippmann-Schwinger equation (LS) has been widely applied to investigate non-equilibrium electron transport and thermoelectric properties in the nanoscale junctions. In this talk, we will briefly present an introduction for DFT+LS theory for the nanoscale junctions formed by atoms/molecule sandwiched between bimetallic electrodes (modeled as electron jellium) with semi-infinite planar surface. We then focus on how we apply LS+DFT to investigate the thermoelectric properties and the current-induced effects from first-principles approaches. We will discuss the following subtopics: (1) nonlinear current-voltage characteristics; (2) gate-controllable current in single-molecule transistors; (3) current-induced force; (4) shot noise; (5) counting statistics; (6) local heating; (7) inelastic electron tunneling spectroscopy (IETS); (8) thermoelectricity and the energy-conversing mechanism between thermal and electric current; and (9) atomic-scale thermoelectric devices, such and nano-refrigerators, power generators, and self-powered electronic nano-devices.

【參考文獻】/ References:

[1] Chun-Lan Ma, Diu Nghiem, and Y-.C. Chen*, Appl. Phys. Lett. **93**, 222111 (2008).
[2] Y. S. Liu and Y.-C. Chen*, Phys. Rev. B. **79**, 193101 (2009).
[3] Y. S. Liu, Y. R. Chen and Y.-C. Chen*, ACS Nano **3**, 3497 (2009)
[4] Y. S. Liu, Bailey C. Hsu, and Y.-C. Chen*, J. Phys. Chem. C **115**, 6111 (2011).
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[6] Y. S. Liu and Y.-C. Chen*, Phys. Rev. B **83**, 035401 (2011).
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二、與會心得

(1) APS MMarch Meeting 會議中遇見 Unisercity of California 的 Prof. Di Ventra，談了一些是否將來可以在 NDA Memory 系統的研究合作。在演講的 section，也遇到 Uiversity of McGill, Canada 的 Prof. Hong Guo。他在我們那個 Section 有 Invited talk。我們簡略地交換研究心得，Hong Guo 是 DFT+nonequiliburin Green's function transport code 的先驅，和我們的研究方式不同但等價。他和香港大學的王健教授合作，最近也計算了奈米接面的量子噪音。和我們的 counting statistics 密切相關。
(2) 在"量子輸運理論和納米電子學模擬國際研討會"中，我在前半段的會議中有 30 分鐘的邀請報告。在後半段的會議中，有一個 90 分鐘的講座。在會議中，強烈感受到大陸最近在基礎科學研究上的長足進步與強烈的企圖心和蓬勃發展。我們應該惕勵自己不能被超越而落後。

三、考察參觀活動(無是項活動者略)

四、建議

五、攜回資料名稱及內容

APS March Meeting Catalog.

六、其他