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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)

奈米接面系統的簡併電子與磁自旋電子的輸運性質

(1/3)

計畫類別： 個別型計畫 整合型計畫

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計畫主持人：陳煜璋

共同主持人：

計畫參與人員：劉玉申(博士後)

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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

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國際合作研究計畫國外研究報告書一份

I. 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。

我們目前的研究重心在探討 molecular junction 的熱電效應與電子自旋效應，我們同時也研究電子輸運性質的多體效應、例如電聲子交互作用與高階 Shot noise 等研究課題。這些研究工作需要開發新的理論與程式，難度比較高。分子電子學是一個國際競爭非常激烈，進步非常快速的研究領域。時間是研究的競爭力和影響力的重要決定因素之一。我們將研究重心朝著此領域中較新穎的研究課題方向發展，希望能夠在前沿課題的研究競爭中取得領先的地位。提升我們的研究影響力與新穎性。

II. 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。傳統電子學的理论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。可被重覆量測驗證的系統(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 上發表分子界面系統的熱電效應，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。

III. 部分研究成果與討論

我們以密度泛函理論，第一原理計算的方式研究原子分子尺度下，奈米界面系統的電子輸運性質與熱電效應。包含電流-電壓特徵曲線關係的探討和電流所引起產生的相關多體效應。進行中的工作方向如下：

- (1) 研究奈米界面系統的熱電效應與電聲子相互作用對熱電效應的影響。
- (2) 研究高階電流量子噪音在氫分子界面系統中的作用與影響，。
- (3) 研究電子自旋對分子界面系統電子輸運的影響。

其中第(1)部分的理論推倒程式撰寫與數值計算已經完成，在熱電效應 Seebeck coefficient 部分，他延續上一年度國科會計畫所聘請的馬春蘭博士硫氫烷醇(Alkanethiol) 分子為的密度泛函理論計算為基礎，研發出全新的理論架構，結合第一原理計算，可以應用於分子界面系統的 Seebeck coefficient 的研究，已經完成一篇論文(Phys. Rev B 79, 193101 (2009).) 接受。我們並且進一步探討此系統的 electron quantum transport 和 phonon quantum transport。進一步研究奈米界面系統的 thermoelectric figure of merit、熱電轉換效率與電聲子交互作用的影響。目前已完成兩篇 manuscripts: arXiv:0902.3876 與 arXiv:0904.0692 (目前 manuscript submitted to PRL); 第(2)部分奈米界面的三階量子噪音的理論推導過程已經接近完成階段，即將進入數值計算工作，我們已經計算了氫分子在 Pt 界面中的電導和 shot noise，再另外他推廣我們以前對二階量子噪音的理論計算到三階量子噪音，該理論計算非常繁雜，需要檢驗近一千項的貢；第(3)部分因為自旋的引進需要整個 DFT 城市的改寫，比較複雜，需要比較龐大的程式撰寫與修改，困難度很高，目前仍然在努力當中。我們僅在此簡述第(1)部分的部分結果。

Part I: Thermoelectricity in Nanojunction:

Title: **Seebeck coefficient of thermoelectric molecular junctions: First-principles calculations**

Authors: Yu-Shen Liu and Yu-Chang Chen*

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Abstract:

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.

The purpose of molecular electronics is to develop a new type of electronic device based on molecules. Understanding the charge transport in metal-molecule-metal (m-M-m) tunnel junctions is of fundamental interest motivated by both scientific challenge and technological importance in subminiature devices. Much attention has been devoted to investigate the various transport properties that might be applicable to develop new forms of electronic and energy-conversion devices such as electron transfer, shot noise, heat transport, negative differential resistance, and gate-controlled effects. Another important property of electron transport in (m-M-m) tunnel junctions is the thermal power (thermoelectricity). The study of thermoelectricity in molecular junctions is of key importance in the design of novel thermo-related electronic and energy-conversion devices at the atomic and molecular level. While thermoelectricity in atomic wires was studied a few years ago, research focusing on the Seebeck coefficient in the molecular system has been conducted only recently.

Considering an m-M-m tunnel junction that may have different temperatures in the source and drain electrodes, a small thermoelectric voltage (ΔV) in the junctions can be induced by an additional temperature difference (ΔT) applied in the electrodes. The ratio of the thermoelectric voltage to the temperature difference is defined as the Seebeck coefficient. The Seebeck coefficient may provide further insights into the physical properties of the molecular tunnel junctions. For example, whether the Fermi energy is closer to the lowest unoccupied molecular orbital (LUMO) or the highest occupied molecular orbital (HOMO) may be locally probed via thermoelectricity measurements⁵. Motivated by recent experimental and theoretical studies on the topic of thermoelectricity in the molecular junction, we investigated the Seebeck coefficient of a single molecule in the two-terminal and three-terminal junctions from first-principles approaches. Particularly, we studied the alkanethiol ($\text{CH}_3(\text{CH}_2)_{n-1}\text{SH}$, denoted as C_n)-related molecules as an example. Alkanethiols are a good representation of reproducible junctions that can be fabricated⁹⁻¹¹. It has been established that non-resonant tunneling is the main conduction mechanism as the Fermi levels of the two electrodes lie within the large HOMO-LUMO gap. However, functional group substitution may have significant effects on the electronic structures of alkanethiols. It is interesting to observe that a new molecular orbital between the HOMO-LUMO gap is produced when $-\text{NH}_2$ is substituted for $-\text{H}$ in bridging butanethiol (C_4), the result of which leads to resonant tunneling in the amino-substituted junction. Due to the dramatic change in the density of states (DOSs) by amino substitution, the novel characteristics of the Seebeck coefficient are observed in the amino-substituted junction. We focused on the comparison of the Seebeck coefficient between amino-substituted and unsubstituted junctions in the two- and three-terminal geometries. We observed that amino substitution significantly affects the Seebeck coefficient. For example, the Seebeck coefficient can change signs by applying gate voltages in the amino-substituted junction but not in the unsubstituted

system. The influence of the temperature gap between the two electrodes on the Seebeck coefficient, controllable by the gate voltages, is significant in the amino-substituted junction. Our results suggest that thermoelectric molecule devices such as a molecular thermometer are possible in the future.

In this paper, we investigate the dependence of the Seebeck coefficient on the source-drain biases, gate voltages, and temperatures in the metal electrodes before and after amino substitution in the butanethiol molecular junction.

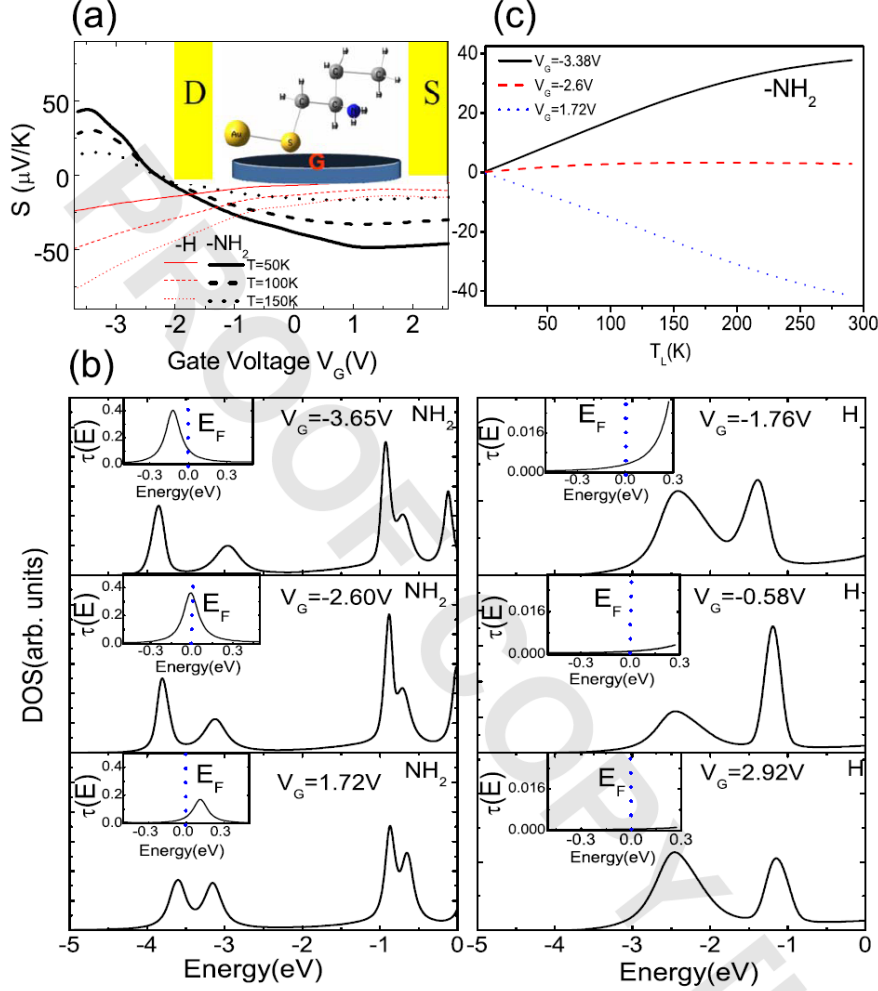


FIG. 1. (Color online) The Seebeck coefficient S in a three-terminal geometry with $V_{SD}=0.01\text{ V}$: (a) S versus V_G where $T_L = T_R = T$ for the amino-substituted [black (thick) lines] and unsubstituted [red (thin) lines] butanethiol for $T=50\text{ K}$ (solid line), $T=100\text{ K}$ (dashed line), and $T=150\text{ K}$ (dotted line). The inset shows the schematic of the three-terminal junction. The gate field is applied in a direction perpendicular to the direction of charge transport. (b) The density of states and the transmission function (inset): the left panels for the amino-substituted butanethiol junction at $V_G = -3.65, -2.60,$ and 1.72 V ; the right panels are for the unsubstituted butanethiol junction at $V_G = -1.76, -0.58,$ and 2.92 V . (c) S versus T_L for an amino-substituted butanethiol junction for $V_G = -3.38, -2.60,$ and 1.72 V , where $T_R = 0\text{ K}$.

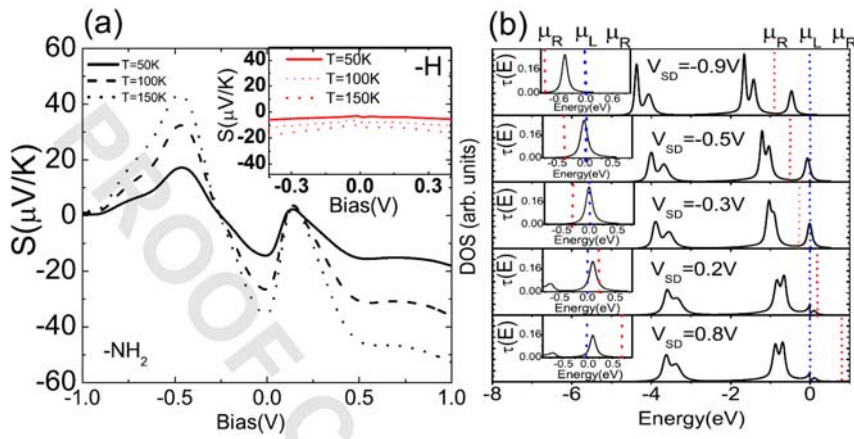


FIG. 2. (Color online) (a) The Seebeck coefficient S as a function of source-drain biases in a two-terminal geometry for amino-substituted (main graph) and unsubstituted (inset in the upper right corner) butanethiol for $T = 50$ K (solid lines), $T = 100$ K (dashed lines), and $T = 150$ K (dotted lines). (b) The density of states and the transmission function (inset) for various source-drain biases ($V_{SD} = -0.9, -0.5, -0.3, 0.2,$ and 0.8 V) in the amino-substituted butanethiol junction.

The study investigates the thermoelectricity in the molecular junction in both linear and nonlinear regimes. The Seebeck coefficients are studied using first-principles calculations. The general properties of the Seebeck effects can be very different for the unsubstituted and aminosubstituted butanethiol junctions in the two-terminal and three-terminal molecular geometries. The research illustrates that the gate field is able to modulate and optimize the Seebeck coefficient. Another interesting phenomenon is the possibility to change the signs of the Seebeck coefficient by applying the gate voltages and biases in amino-substituted butanethiol junction. It is observed that the Seebeck coefficient is relevant to the temperatures of the electrodes that may be applied to the design of a molecular thermometer and its sensibility can be controlled by gate voltages. We also extend the investigation of the Seebeck coefficient to molecular tunnel junction at finite biases. 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. All results show that the molecular tunnel junction based on alkanethiols may be a promising candidate for the design of novel thermoelectric devices in the future.

Title: Do Thermoelectric Materials in Nanojunctions Display Material Property or Junction Property?

Authors: Yu-Chang Chen* and Yu-Shen Liu

Abstract:

Do Thermoelectric Materials in Nanojunctions Display Material Property or Junction Property?

By Yu-Chang Chen (陳煜璋) Yu-Shen Liu (劉玉申)

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 cancelation of exponential scalings in the DOSs. For ZT , the atomic wires remain to show strong junction properties. However, the length characteristics of the insulating molecular wires depend on a characteristic temperature T_0 around 10 K. When $T \ll T_0$, where the electron transport dominates the thermal current, the molecular junctions remain to show material properties. When $T \gg T_0$, where the phonon transport dominates the thermal current, the molecular junctions display junction properties.

Indeed, the miniaturization of thermoelectric nanojunctions raises a fundamental question: does bridging thermoelectric material in nanojunctions show material properties or junction properties? Thermoelectric bulk crystals usually show material properties, where the thermoelectric physical quantities are irrelevant to the sizes and shapes of materials. In addition, recent experiments on Seebeck coefficients in molecular junctions also reveal strong signals of material properties. These experiments have observed that Seebeck coefficients are insensitive to the number of molecules in junctions and show rather weak dependence on the lengths of the bridging molecules, which is in sharp contrast to the conductance which shows strong exponential dependence on the lengths of molecules [11–13]. However, the bridging materials in nanojunctions may have strong interactions with the contacts. From this point of view one can say thermoelectric quantities can display the junction characteristics. Considering the examples and the reason quoted above, it is therefore not obvious whether the thermoelectric quantities of the bridging materials in nanojunctions display junction properties or material properties.

The miniaturization of thermoelectric junctions generates new Physics due to quantum transport for electrons and phonons at atomic levels. In this letter, we will show that the thermoelectric quantities in nanojunctions unnecessarily display entire material properties or junction properties. To demonstrate this point, this study investigates two important thermoelectric quantities, the Seebeck coefficient (S) and the thermoelectric figure of merit (ZT), in (metallic) aluminum atomic junctions and (insulating) molecular junctions. It shows that metallic atomic chains reveal strong junction properties while the insulating molecular wires partially possess the material properties, where S reveals the material property and ZT displays the junction property at temperatures larger than the characteristic temperature T_0 .

To answer the question, we have developed a theory with analytical expressions for S and ZT allied to a fully self-consistent first-principles calculation in the framework of the

densityfunctional theory (DFT).

(detailed content please see ArXive: 0904.0692)

98 年度自然處專題計畫主持人近五年研究成果

(修正：98/03/27)

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(一)、近五年內(2003/1/1~2009/12/31)最具代表性研究成果至多六篇。

(請依序填寫：姓名,發表年份,著作名稱,期刊,卷數,頁數,並以*號註記該篇之通訊作者)

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4. “Inelastic current-voltage characteristics of atomic and molecular junctions.”
Nano Lett. **4** 1709 (2004).
Y.-C. Chen, M. Zwolak, and M. Di Ventra
5. “Local Heating in Nanoscale conductors.”
Nano Lett. **3** 1691 (2003); *ibid* **5**, 813 (2005).
Y.-C. Chen, M. Zwolak, and M. Di Ventra
6. “Shot Noise in Nanoscale Conductors From First Principles.”
Phys. Rev. B **67** 15304 (2003).
Y.-C. Chen and M. Di Ventra

(二)、近五年內獲獎情形及重要會議邀請演講至多五項。

(A) Invited talks in international conference:

- [1]. Mesoscopic and Spin Physics Novel Quantum Phenomena in Condensed Matter: The topic program on Superconductivity and Magnetism at Nanoscale: Effects of quantum fluctuations and disorder, Hsinchu, Taiwan, Dec17-19, 2007.
“Isotope Effects in the Hydrogen Molecular Junctions”
- [2]. Computational Methods in Materials Research and Development (CMM) under MP3-2007 (The 6th International Conference on Materials Procession, Properties and Performance), Beijing, China, Sept. 13-16, 2007.
“Isotope Effects in the Hydrogen Molecular Junctions”
- [3]. The 5-th Joint Meeting of the Chinese Physicists Worldwide International Conference On Physics Education and Frontier Physics. Taipei. June 27-30, 2006.
“Inelastic Effects on the Transport Properties in Nano Junction.”

[4]. Workshop on Mesoscopic and Spin Physics 2006, National Chiao Tung University, Jan. 5-7, 2006.

“Inelastic Effects on Current and Shot Noise in Nanoscale Junctions.”

[5]. The 8th Asian Workshop on First-Principles Electronic Structure Calculations, Shanghai, China, Oct.31-Nov.2, 2005.

“Effects of electron-phonon scattering on shot noise in nanoscale junctions.”

[6]. Materials Research Society Spring Meeting, San Francisco, CA, USA, April. 22-24, 2003.

“Heating and fluctuation in nanoscale conductors from first principle.”

(三)、近五年內其他資料 (如：擔任國際重要學術學會理監事、國際知名學術期刊編輯或評審委員、專利或技術轉移具體績效等)。

(四)、近五年內重要研究成果簡述。(至多一頁)

[1]. “Alkanethiol-based single-molecule transistors”

Appl. Phys. Letts. 93, XXX (2008) (in press)

Chun-Lan Ma, Diu Nghiem, and Yu-Chang Chen*

Alkanethiol(Cn)分子容易備製，適合作為分子界面電流輸運特性的基礎研究。但該系統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，發現取代後產生新的態，導致不對稱的電流電壓關係曲線。電導也可被開極有效的調控。所以 NH₂ 取代後的 C₄ 分子具有作為分子場效應電晶體的潛力。

[2]. “Measurement of Current-Induced Local Heating in a Single Molecule Junction.”

Nano Lett., 6, 1240 (2006, June).

Z. Huang, B. Xu, **Y.-C. Chen**, M. Di Ventra* and N.J. Tao*

在單一分子所構成的電子元件中，量測到因電流流經由 single molecule junction 所產生的分子元件溫度上升現象。分子元件產生熱的現象是由於電子被分子的振動的散射所產生。實驗結果和第一原理理論計算值符合。

[3]. “Effect of electron-phonon scattering on shot noise in nanoscale junctions.”

Phys. Rev. Lett., 95, 166802 (2005, October).

Y.-C. Chen* and M. Di Ventra*

在原子分子尺度下，探討 nanojunction 中 shot noise(即在絕對零度時電流的量子漲落現象)受到電聲子散射所造成的影響。此量子效應的研究有助於關於電聲子散射對奈米界面中電子傳輸基本的量子干涉行為的基本物理機制的了解。

[4]. “Inelastic effect on the transport properties of alkanethiols.”

Nano Lett., 5, 621 (2005, March).

Y.-C. Chen, M. Zwolak, and M. Di Ventra*

探討 alkanethiol nanojunction 中的傳輸電子和分子振動的交互作用對電流電壓關係曲線的影響。發現 I-V characteristics 二次微分的峰值大小和分子震動在電流方向上的分量大小有關，也和 C 原子數目的奇偶數有關。計算和 IETS 以及 HREELS 實驗所測量的實驗結果相符合。

[5]. “Local Heating in Nanoscale conductors.”

Nano Lett. **3** 1691 (2003, October).

Y.-C. Chen, M. Zwolak, and M. Di Ventra*

在原子分子尺度下該論文是文獻上第一篇以第一原理方法(電子密度泛函)計算奈米界面中電流對奈米界面產生的溫度加熱效應。分子電子元件的溫度對電子元件的穩定度和電子元件的效率有重要的影響。

[List of Publication]

1. Title: Seebeck coefficient of thermoelectric molecular junctions: First-principles calculations
Author(s): Liu,YS; CHEN, YC
Source: **PHYSICAL REVIEW B** Volume: 79 Issue: 19 Pages: 193101 Published: **MAY 15 2009**
Times Cited: **32**
2. Title: Alkanethiol-based single-molecule transistors
Author(s): MA, CL; NGHIEM, D; CHEN, YC
Source: **APPLIED PHYSICS LETTERS** Volume: 93 Issue: 22 Pages: 222111 Published: **2008**
Times Cited: **0**
3. Title: Effects of isotope substitution on local heating and inelastic current in hydrogen molecular junctions
Author(s): CHEN, YC
Source: **PHYSICAL REVIEW B** Volume: 78 Issue: 23 Pages: 233310 Published: **2008**
Times Cited: **0**
4. Title: Effect of atomic geometry on shot noise in aluminum quantum point contacts
Author(s): YAO, J; CHEN, YC; DI VENTRA, M; et al.
Source: **PHYSICAL REVIEW B** Volume: 73 Issue: 23 Pages: 233407 Published: **2006**
Times Cited: **1**
5. Title: Measurement of current-induced local heating in a single molecule junction
Author(s): HUANG, ZF; XU, BQ; CHEN, YC; et al.
Source: **NANO LETTERS** Volume: 6 Pages: 1240-1244 Published: **2006**
Times Cited: **40**
6. Title: Effect of electron-phonon scattering on shot noise in nanoscale junctions
Author(s): CHEN, YC; DI VENTRA, M
Source: **PHYSICAL REVIEW LETTERS** Volume: 95 Issue: 16 Pages: 166802 Published: **OCT 14 2005**
Times Cited: **16**
7. Title: Inelastic current-voltage characteristics of atomic and molecular junctions. (vol 4, pg 1710, 2004)
Author(s): CHEN, YC; ZWOLAK, M; DI VENTRA, M
Source: **NANO LETTERS** Volume: 5 Issue: 4 Pages: 813 Published: **APR 2005**

Times Cited: 0

8. Title: Inelastic effects on the transport properties of alkanethiols

Author(s): CHEN, YC; ZWOLAK, M; DI VENTRA, M

Source: **NANO LETTERS** Volume: 5 Pages: 621-624 Published: 2005

Times Cited: 39

9. Title: Role of heating and current-induced forces in the stability of atomic wires

Author(s): YANG, Z; CHSHIEV, M; ZWOLAK, M; et al.

Source: **PHYSICAL REVIEW B** Volume: 71 Issue: 4 Pages: 041402(R) Published: JAN 2005

Times Cited: 32

10. Title: Are current-induced forces conservative?

Author(s): DI VENTRA, M; CHEN, YC; TODOROV, TN

Source: **PHYSICAL REVIEW LETTERS** Volume: 92 Issue: 17 Pages: 176803 Published: APR 30 2004

Times Cited: 24

11. Title: Inelastic current-voltage characteristics of atomic and molecular junctions

Author(s): CHEN, YC; ZWOLAK, M; DI VENTRA, M

Source: **NANO LETTERS** Volume: 4 Issue: 9 Pages: 1709-1712 Published: SEP 2004

Times Cited: 49

12. Title: Shot noise in parallel wires

Author(s): LAGERQVIST, J; CHEN, YC; DI VENTRA, M

Source: **NANOTECHNOLOGY** Volume: 15 Issue: 7 Pages: S459-S464 Published: JUL 2004

Times Cited: 8

13. Title: Local heating in nanoscale conductors

Author(s): CHEN, YC; ZWOLAK, M; DI VENTRA, M

Source: **NANO LETTERS** Volume: 3 Issue: 12 Pages: 1691-1694 Published: DEC 2003

Times Cited: 74

14. Title: Shot noise in nanoscale conductors from first principles

Author(s): CHEN, YC; DI VENTRA, M

Source: **PHYSICAL REVIEW B** Volume: 67 Issue: 15 Pages: 15304 Published: APR 15 2003

Times Cited: 18

15. Title: Diluted quantum antiferromagnets: Spin excitations and long-range order

Author(s): CHERNYSHEV, AL; CHEN, YC; NETO, AHC

Source: **PHYSICAL REVIEW B** Volume: 65 Issue: 10 Pages: 104407 Published: MAR 1 2002

Times Cited: 32

16. Title: Effect of impurities on quasi-two-dimensional quantum antiferromagnet

Author(s): CHERNYSHEV, AL; CHEN, YC; NETO, AHC

Source: **JOURNAL OF APPLIED PHYSICS** Volume: 91 Issue: 10 Pages: 8387-8389 Published: 2002

Times Cited: 0

17. Title: Long-range order and low-energy spectrum of diluted 2D quantum antiferromagnet
 Author(s): CHERNYSHEV, AL; CHEN, YC; NETO, AHC
 Source: **PHYSICAL REVIEW LETTERS** Volume: 87 Issue: 6 Pages: 067209 Published: **AUG 6 2001**
 Times Cited: 10
18. Title: Effective field theory for layered quantum antiferromagnets with nonmagnetic impurities
 Author(s): CHEN, YC; NETO, AHC
 Source: **PHYSICAL REVIEW B** Volume: 61 Issue: 6 Pages: R3772-R3775 Published: **FEB 1 2000**
 Times Cited: 16

統計類別	2004		2005		2006		2007		2008	
	總篇數	IF 總和	總篇數	IF 總和	總篇數	IF 總和	總篇數	IF 總和	總篇數	IF 總和
所有SCI期刊論文(含共同作者)	3	19.931	3	19.793	2	12.799	0	0	2	6.768
SCI期刊論文(限通訊作者)					1	6.994			2	6.768
其他著作	1. 專書：___件、 2. 專利或技轉：___件									

說明：

- 請依照個人資料表所列之研究成果，於上表提供五年內(2002/1/1~2006/12/31)已發表或被接受發表於SCI期刊、專書、專利或技術移轉等資料。
- SCI (Science Citation Index) 之 **Impact Factor** 係以 **2005 年版本為準**。請至有購買 Journal Citation Reports on the Web，簡稱 JCR Web，資料庫之各大學圖書館或財團法人國家實驗研究院科技政策研究與資訊中心 (<http://www.stic.gov.tw/fdb/jcr/index.html>) 進行查詢。
- IF 總和：係該年度論文所刊載期刊之 Impact Factor 總和。

處理方式：除產學合作研究計畫、提升產業技術及人才培育研究計畫、
列管計畫及下列情形者外，得立即公開查詢
 涉及專利或其他智慧財產權， 一年 二年後可公開查詢

執行單位：交通大學電子物理系

中 華 民 國 98 年 5 月 6 日

附件二

可供推廣之研發成果資料表

可申請專利

可技術移轉

日期：__年__月__日

國科會補助計畫	計畫名稱： 計畫主持人： 計畫編號： 學門領域：
技術/創作名稱	
發明人/創作人	
技術說明	中文： <div style="text-align: center;">(100~500 字)</div>
	英文：
可利用之產業 及 可開發之產品	

技術特點	
推廣及運用的價值	

- ※ 1. 每項研發成果請填寫一式二份，一份隨成果報告送繳本會，一份送 貴單位研發成果推廣單位（如技術移轉中心）。
- ※ 2. 本項研發成果若尚未申請專利，請勿揭露可申請專利之主要內容。
- ※ 3. 本表若不敷使用，請自行影印使用。