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二、內容格式：依序為封面、中英文摘要、目錄（精簡報告得省略）、報告內容、參考文獻、計畫成果自評、可供推廣之研發成果資料表、附錄。

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(三)報告內容：請包括前言、研究目的、文獻探討、研究方法、結果與討論（含結論與建議）…等。若該計畫已有論文發表者，可以 A4 紙影印，作為成果報告內容或附錄，並請註明發表刊物名稱、卷期及出版日期。若有與執行本計畫相關之著作、專利、技術報告、或學生畢業論文等，請在參考文獻內註明之，俾可供進一步查考。

(四)頁碼編寫：請對摘要及目錄部分用羅馬字Ⅰ、II、 III……標在每頁下方中央；報告內容至附錄部分請以阿拉伯數字 1.2.3.……順序標在每頁下方中央。

(五)附表及附圖可列在文中或參考文獻之後，各表、圖請說明內容。

(六)計畫成果自評部份，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、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。

(七)可供推廣之研發成果資料表：凡研究性質屬***應用研究***及***技術發展***之計畫，請依本會提供之表格（如附件二），每項研發成果填寫一份。

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1. 用紙

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報告之正文以中英文撰寫均可。在字體之使用方面，英文使用 Times New Roman Font，中文使用標楷體，字體大小請以 12 號為主。

附件一

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

(2/3)

計畫類別：■ 個別型計畫　□ 整合型計畫
計畫編號：97-2112-M-009-011-MY3
執行期間：　2008 年 8 月 1 日至　2011 年 7 月 31 日

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)
碩士班研究生:陳譯仁、翁廷達、包智傑、姚宣德、曾怡仁、陳彥廷

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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□赴國外出差或研習心得報告一份
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■出席國際學術會議心得報告及發表之論文各一份
□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。

III. 部分研究成果與討論

我們研究方式是以密度泛函理論結合量子多體理論，第一原理計算的方式研究原子分子尺度下，奈米接面系統的電子輸運性質，自旋電子特性與熱電效應。研究的主題包含電流-電壓特徵曲線、隧穿電子和分子震盪交互作用引起的 inelastic electron tunneling spectroscopy（IETS）與侷域熱生成(local heating)、電流量子化產生的量子噪音。最近的重心則擺在分子接面系統的熱電性質，包含聲子的熱流與新型態分子熱電元件的理論研究。另一重點則是分子自旋電子學的理論研究。進行中的工作方向如下：

（1）研究奈米接面系統的熱電效應與電聲子交互作用對對熱電效應的影響。

（2）研究高階電流量子噪音在氫分子接面系統中的作用與影響，。

（3）研究電子自旋對分子接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，我們延續上一年度國科會計畫硫氫烷醇(Alkanethiol)分子為的密度泛函理論計算為基礎(Chun-Lan Ma, Diu Nghiem, and Y-.C. Chen* Appl. Phys. Lett. 93, 222111 (2008).)，研發出全新的分子接面系統理論架構，結合第一原理數值計算，應用於的 Seebeck coefficient 與 figure of merit (ZT) 的研究，目前已經完成兩篇論文 發表在 Phys. Rev B (Y. S. Liu and Y. C. Chen* Phys. Rev. B 79, 193101 (2009). 與 ACS Nano (Y. S. Liu, Y. R. Chen and Y. C. Chen*, ACS Nano 3, 3497 (2009).)。關於熱電效應元件的應用，我們提出以原子接面系統作為致冷機，論文初稿已經完成(cond-mat/arXiv:0908.0992)與 Power generator (cond-mat/arXiv:1001.0822)，目前正在投稿與審稿階段。劉玉申和我的前研究生翁廷達與包智傑合作，完成關於苯環分子官能基取代後的電子輸運性質、Seebeck coefficient 與 power factor 的研究。目前已經在整理最後數據與撰稿階段，近期內會完成並整理成為三篇論文投稿。

在奈米接面的三階量子噪音的研究方面，我們也完成了碳原子鍊的二階與三階 quantum current correlation 的研究。該論文將是文獻上首次出現關於分子接面系統的的高階量子噪音的研究。目前該論文已經完成並正在做最後的校稿與潤稿，我們即將投稿至 PRL。

在電聲子交互作用對 Seebeck coefficient 的影響的研究方面，我們也已經完成理論推導與程式撰寫，與大部分的電腦程式計算工作。該項工作也即將完成，已經進入部分論文草稿階段。

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)與(2)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*

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

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 measurements[5]. 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 ($CH_3(CH_2)_{n-1}SH$, 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 $–NH_2$ is substituted for –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.

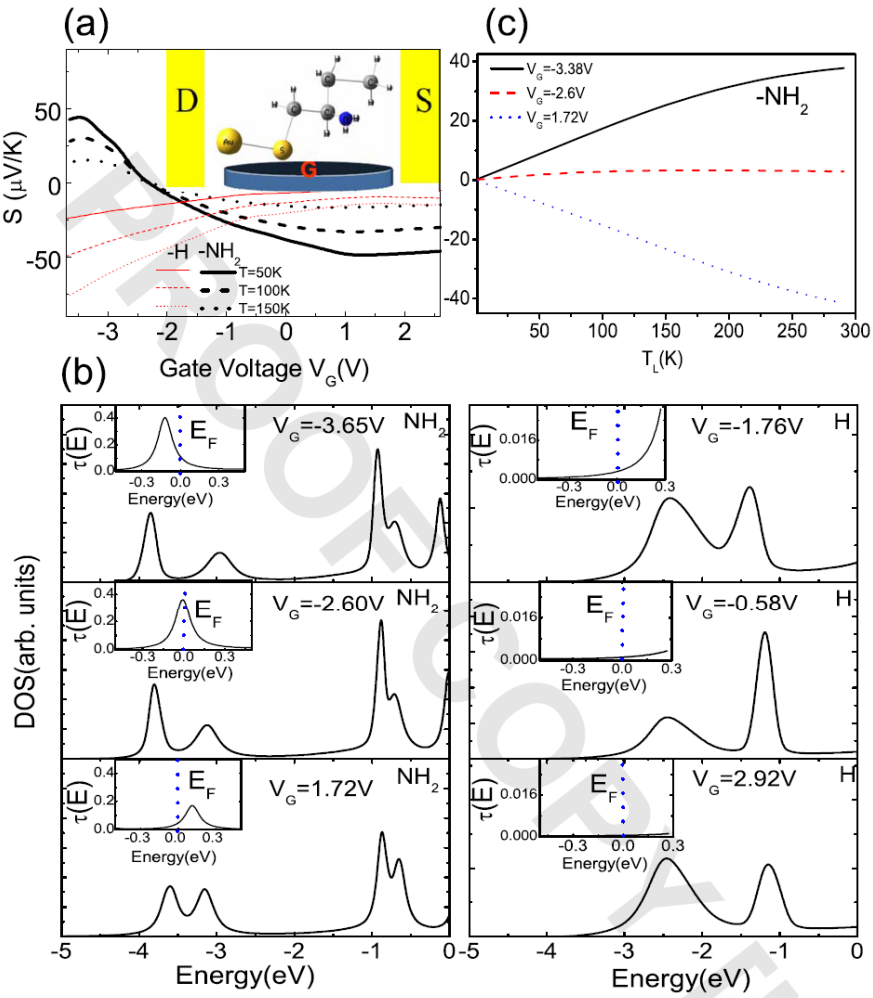


FIG. 1. (Color online) The Seebeck coefficient S in a three-terminal geometry with $V_{SD}=0.01$ V: (a) S versus V_G where $T_L=T_R=T$ for the amino-substituted [black (thick) lines] and unsubstituted [red (thin) lines] butanethiol for $T=50$ K (solid line), $T=100$ K (dashed line), and $T=150$ K (dotted line). The inset shows

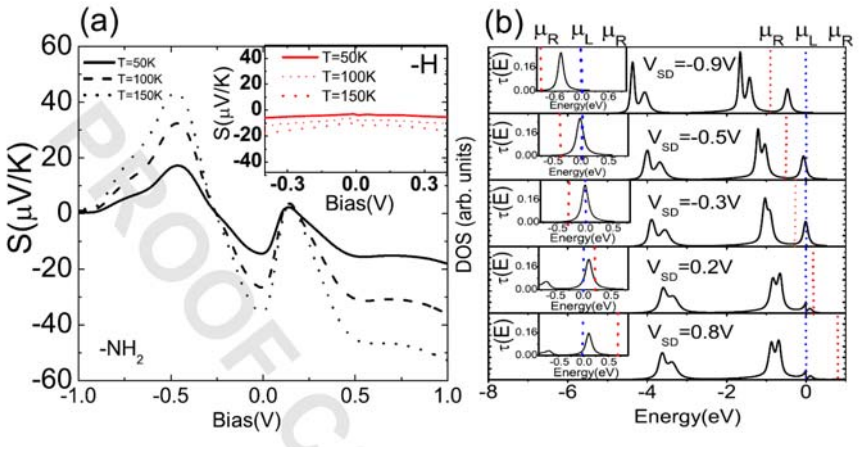


FIG. 2. (Color online) (a) The Seebeck coefficient S as a function of source-drain biases in a two-terminal geometry for amino-substituted (main graph) and unsubstituted (inset in the upper right corner) butanethiol for $T=50$ K (solid lines), $T=100$ K (dashed lines), and $T=150$ K (dotted lines). (b) 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 firstprinciples 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 JunctionProperty?

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 chrematistics of the insulation 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 ($\mathcal{S}$) 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)

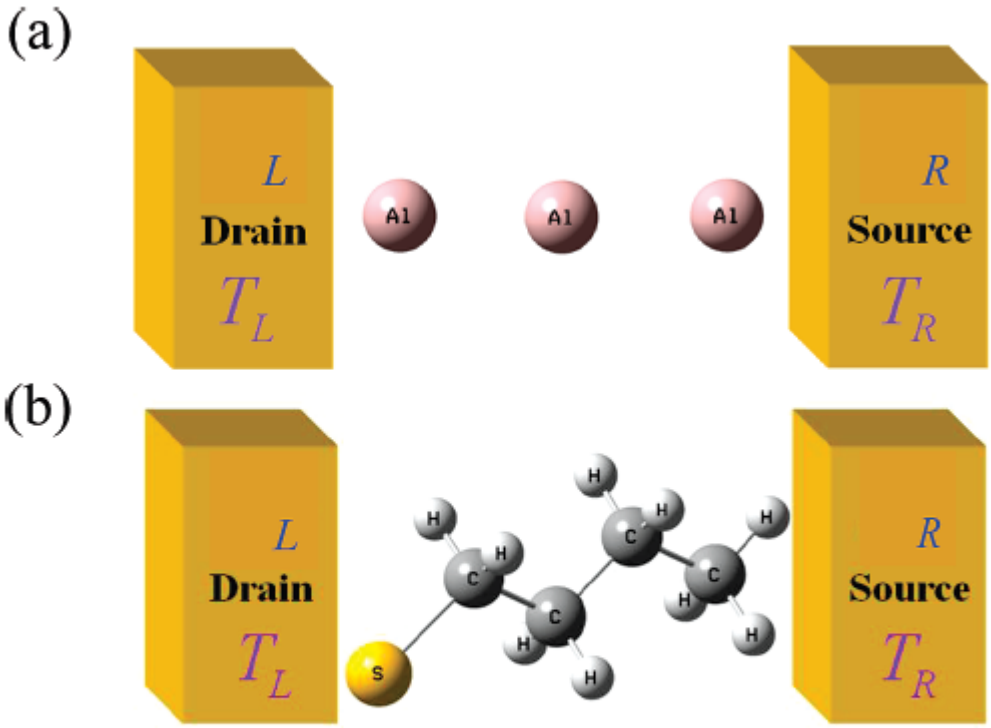
Title: Thermoelectric Efficiency in Nanojunctions: A Comparison between Atomic Junctions and Molecular Junctions

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

Published in ACS Nano 3, 3497 (2009).

ABSTRACT:

Using the 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 thermal current carried by electrons and phonons. We also observe a characteristic temperature: $T_0 = \sqrt{\beta / \gamma(l)}$. When $T \ll T_0$, the electronic heat current dominates the combined thermal current and $ZT \propto T^2$. When $T \gg T_0$, the phononic heat current dominates the combined thermal current and ZT, which lean toward a saturation value. Moreover, the metallic atomic junctions and the insulating molecular junctions have an 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 molecular junctions.



Scheme 1. Schemes of the systems investigated: (a) the 3-Al atomic junction and (b) the C_4 molecular junction. Two bulk electrodes are modeled as independent electron reservoirs with distinct chemical potentials $\mu_{L(R)}$ and distinct temperatures $T_{L(R)}$.

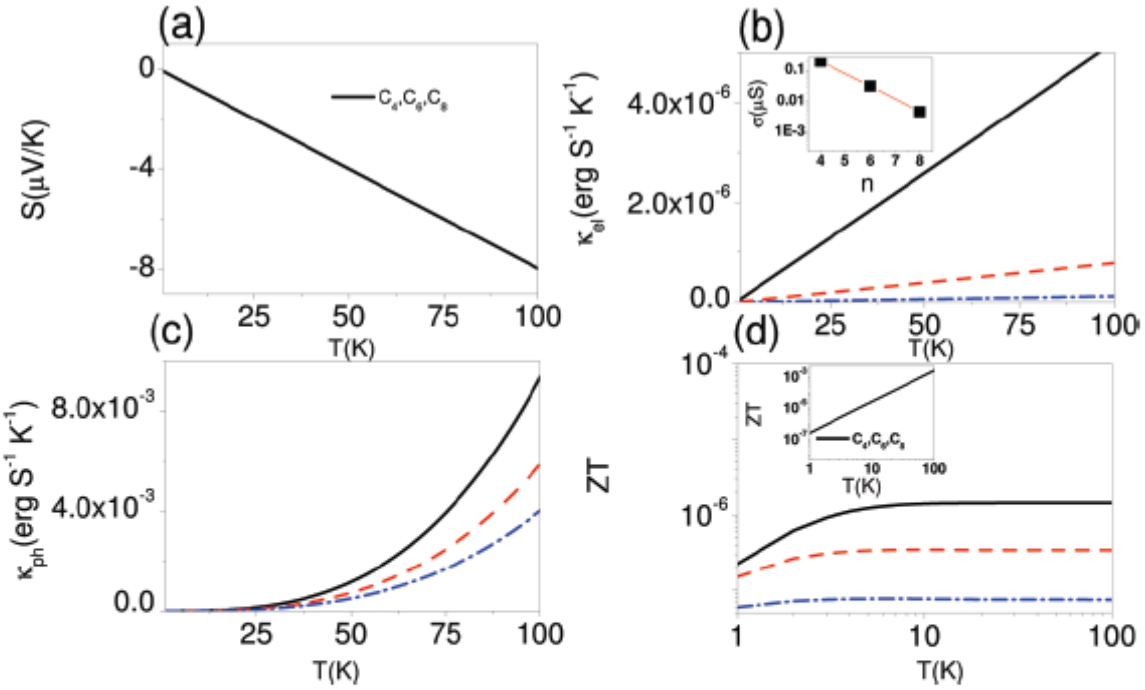


Figure 2. Alkanethiol junctions at $V_B = 0$ V for C_4 (solid black lines), C_6 (dashed red lines), and C_8 (dot-dashed lines). (a) Seebeck coefficient S as a function of T. (b) Electronic heat conductance κ_{el} as a function of T. Inset shows semi-log of electric conductance σ as a function of n, where n is the number of carbon atoms. (c) Phononic heat conductance κ_{ph} as a function of T. (d) Log−log of ZT as a function of T. Inset shows the case of neglecting of the phononic heat conductance $\kappa_{ph} = 0$.

In conclusion, the self-consistent DFT calculations together with analytical expressions are applied to investigate the thermoelectric figure of merit ZT in the nanoscale junctions. There is a characteristic temperature T_0 for ZT, which his defined as the temperature where the electronic heat conductance equals the phononic heat conductance. When $T \ll T_0$, the electronic heat conductance dominates the combined thermal conductance and $ZT \propto \left(\alpha^2\sigma / \beta\right)T^2$; when $T \gg T_0$, the phononic heat conductance dominates the combined thermal conductance and ZT, which leads to the saturation value $\alpha^2\sigma / \gamma(l)$.

The relation between ZT and the lengths of nanojunction depends on the conducting mechanism: for aluminum atomic (conducting) wires, the saturation value of ZT increases as the length increases, owing to $k_{ph} \propto l^{-2}$ which dominates the length-dependence; while for the alkanethiol (insulating) chains, the saturation value of ZT decreases as the length increases owing to $\sigma \exp\left(-\xi l\right)$ which dominates the length-dependence. Thus, the dependence of ZT on the lengths for the metallic atomic junctions is opposite to that for the insulating molecular junctions. In addition, we also find that T_0 of the aluminum atomic (conducting) junction increases as the length of the junction increases; on the other hand, T_0 of the alkanethiol (insulating) junction decreases as the length of the junction increases. The difference in the length-dependence between the insulation molecular junctions and the metallic atomic junctions is due to different length-scaling behaviors in the electric conductance.

Of key importance to increasing the thermoelectric efficiency is using materials with a large value of Seebeck coefficient. Such materials are usually characterized by a sharp peak in the transmission function near the Fermi levels. The thermoelectric efficiency could be further optimized by applying gate fields or choosing low-elasticity bridging materials in nanoscale junctions. The widely diversified atomic-sized junctions may be achieved by manipulating the species of nano-structured objects and the contact region. Such manipulations may lead to a significant change in the DOSs, consequently varying the Seebeck coefficient of the nanojunctions. A full exploration of all the possibilities in such an unknown system may lead to observations of large *ZT* values, suitable for practical thermoelectric nanodevices. The conclusions of this study may be beneficial to further studies attempting to increase thermoelectric efficiency through the design of thermoelectric nanodevices at the atomic and molecular levels.

99 年度自然處專題計畫主持人近五年研究成果

（修正：98/10/30）

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(一)、近五年內(2005/1/1～2009/12/31)最具代表性研究成果至多六篇，擇五篇電子檔上傳。（請依序填寫：姓名, 發表年份, 著作名稱, 期刊, 卷數, 頁數, IF，並以*號註記該篇所有的通訊作者）

1.

Title: Atomistic Thermoelectric Refrigerator: A Proposal via a First-principles Calculation.

Author(s): Yu-Shen Liu and **Yu-Chang Chen***

Submitted to Phys. Rev. Letts.

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

Author(s): Yu-Shen Liu, Yi-Ren Chen and **Yu-Chang Chen***

Source: **ACS Nano** Volume: 3 Pages 3497 Published: November 2009

Times Cited: 0

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

Author(s): Yu-Shen Liu and **Yu-Chang Chen***

Source: **PHYSICAL REVIEW B** Volume: 79 Issue: **19** Pages: **193101** Published: **MAY 2009**

Times Cited: **2**

4. Title: Alkanethiol-based single-molecule transistors

Author(s): Chun-Lan Ma, Diu Nghiem, and **Yu-Chang Chen***

Source: **APPLIED PHYSICS LETTERS** Volume: **93** Issue: **22** Pages: **222111** Published: **December 2008**

Times Cited: **2**

5. Title: Effects of isotope substitution on local heating and inelastic current in hydrogen molecular junctions
Author(s): **Yu-Chang Chen***
Source: **PHYSICAL REVIEW B** Volume: **78** Issue: **23** Pages: **233310** Published: **December 2008**
Times Cited: **1**

6. Title: Effect of atomic geometry on shot noise in aluminum quantum point contacts
Author(s): J. Yao, **Yu-Chang Chen**, M. Diventra, and Z. Q. Yang*
Source: **PHYSICAL REVIEW B** Volume: **73** Issue: **23** Pages: **233407** Published: **June 2006**
Times Cited: **1**

7. Title: Measurement of current-induced local heating in a single molecule junction
Author(s): Zhifeng Huang, Bingqian Xu, **Yu-Chang Chen**, M. Di Ventra*, Nongjian Tao*
Source: **NANO LETTERS** Volume: **6** Pages: **1240** Published: **June 2006**
Times Cited: **51**

8. Title: Effect of electron-phonon scattering on shot noise in nanoscale junctions
Author(s): **Yu-Chang Chen*** and M. Diventra*
Source: **PHYSICAL REVIEW LETTERS** Volume: **95** Issue: **16** Pages: **166802** Published: **OCT 2005**
Times Cited: **19**

9. Title: Inelastic current-voltage characteristics of atomic and molecular junctions. (vol 4, pg 1710, 2004)
Author(s): **Yu-Chang Chen**, M. Zwolak, and M. Di Ventra*
Source: **NANO LETTERS** Volume: **5** Issue: **4** Pages: **813** Published: **APR 2005**
Times Cited: **0**

10. Title: Inelastic effects on the transport properties of alkanethiols
Author(s): **Yu-Chang Chen**, M. Zwolak, and M. Di Ventra*
Source: **NANO LETTERS** Volume: **5** Pages: **621** Published: **APR 2005**
Times Cited: **43**

11. Title: Role of heating and current-induced forces in the stability of atomic wires
Author(s): Z. Yang*, M. Chshiev, M. Zwolak, **Yu-Chang Chen**, M. Di Ventra*
Source: **PHYSICAL REVIEW B** Volume: **71** Issue: **4** Pages: **041402(R)** Published: **JAN 2005**
Times Cited: **35**

（二）、近五年內研究成果統計表

統計類別	2005		2006		2007		2008		2009		以上合計		2009 已接受尚未發表者	
	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	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	20.883	2	13.701	0	0	2	7.058	2	8.804	9	50.446		
SCI 期刊論文（限通訊作者）	1	7.18					2	7.058	2	8.804	5	23.042		
SCI 期刊論文（第一作者，不與上欄重覆計算，僅物理學門須加填寫）	1	10.371									1	10.371		
其他著作	1. 專書：___件、　2. 專利或技轉：___件													

說明：

1. 請依照個人資料表所列之研究成果，於上表提供五年內(2005/1/1～2009/12/31)已發表或被接受(請附證明文件)發表於 SCI 期刊、專書、專利或技術移轉等資料。
2. SCI (Science Citation Index) 之 Impact Factor 係以 2008 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://cdnet.stpi.org.tw/db_search/01_isi.htm)進行查詢。

   IF 總和：係該年度論文所刊載期刊之 Impact Factor 總和。

（三）、近五年內獲獎情形及重要會議邀請演講至多五項。

[1]. Taiwan-Argonne Workshop on Nano-structured Materials Tainan, Taiwan, Feb. 1-2, 2010.
“Thermoelectricity in atomic and molecular junctions”

[2]. The 12th Asian Workshop on First-Principles Electronic Structure Calculations, Beijing, China, Oct.26-28, 2009.
“Thermoelectricity in atomic and molecular junctions”,

[3]. 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”

[4]. 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”

[5]. The 5-th Joint Meeting of the Chinese Physicists Worldwide International Conference On Physics Education and Frontier Physics. Taipei. June 27-30, 2006.
"Inelastic Efeects on the Transport Properties in Nano Junction."
[6]. 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."
[7]. 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."

（四）、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）。

（五）、請簡述上述代表性研究成果內個人之重要貢獻（至多一頁）。

[1]. "Thermoelectric Efficiency in Nanojunctions: A comparison between atomic and molecular junctions."
ACS Nano 3, 3497 (2009)
Yu-Shen Liu, .Yi-Ren Chen and Yu-Chang Chen*

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。

[2]. "Alkanethiol-based single-molecule transistors"
Appl. Phys. Letts. 93, 222111 (2008) (in press)
Chun-Lan Ma, Diu Nghiem, and Yu-Chang Chen*

Alkanethiol(Cn)分子容易備製，適合作為分子接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能態，導致不對稱的電流電壓關係曲線。電導也可被閘極有效的調控。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。

[3]. "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。

[4]. "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接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。

[5]. "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。.