行政院國家科學委員會專題研究計畫 期末報告

電漿子奈米材料之電磁理論與模擬研究

計 畫 類 別 ：個別型
計 畫 編 號 ：NSC 100-2112-M-004-002-
執 行 期 間 ：100 年 08 月 01 日至 101 年 10 月 31 日
執 行 單 位 ：國立政治大學應用物理研究所

計 畫 主 持 人 ：郭光宇

報 告 附 件 ：出席國際會議研究心得報告及發表論文

公 開 資 訊 ：本計畫可公開查詢

中 華 民 國 102 年 01 月 09 日

中文摘要： 表面電漿子是一種侷限在金屬和介質介面的與量子化電子振盪模式強烈耦合的電磁波。表面電漿子的低維特性及增強的介面電磁場引發了各種十分有趣的新奇現象，同時造就了許多新穎的應用如以天文數字般增強的拉曼散射、異常的光通過奈米洞的傳輸、超越光波的繞射極限、改進的太陽能電池效能、微型奈米雷射等。然而，要調控和應用電漿子奈米材料的新穎特性，我們有必要徹底理解決定這些超穎材料物理性質的因子如大小、形狀、成分及環境等。因此，本計畫通過一系列的電磁理論模擬來探討多種奈米材料中表面電漿子相關現象的起因與機理。我們依据所研究系統的特征，採用四種頻域的數值計算方法[格點電偶極近似法(DDA)、多層散射理論(layer KKR)、有限元近似法及平面波展開法]與一種時域的計算方法[即有限差分時域法(FDTD)]. 我們還結合解析的理論方法如改進的長波近似法和異向電偶極模型對各種表面電漿子共振現象的新穎特性質作深入的分析。我們和周遭的實驗同仁交流與合作、努力攻克奈米電漿子學中一些重要研究課題、共同培養奈米光電科技人才。

中文關鍵詞： 電漿子奈米材料、超穎材料、金屬奈米顆粒、光學性質、電磁理論、電磁模擬

英文摘要： The principal purpose of this proposal is to understand the origin and mechanism of the exciting surface plasmon-related phenomena in a range of metal nanomaterials. This has been be achieved primarily by performing extensive numerical electromagnetic simulations. In the past year, we have exploited several complementary frequency-domain methods [e.g., the discrete dipole approximation (DDA) and finite-element, methods] as well as the time-domain method [i.e., finite-difference time domain (FDTD) method)] to investigate the physical properties of a number of novel metamaterials sytems. Indeed, our fascinating and important results have been published in 12 papers in international journals [e.g., very prestigious physics journal Phys. Rev. Lett. (10) and very prestigious nano-science journal Nano Letters (12)] (see the enclosed publication list below) since Aug. 1, 2011. We have also interacted and

collaborated actively with many experimental and theoretical groups at home and abroad. Some research highlights are described in more details below (I). Also enclosed in this report are the list of publications (II) and the list of invited presentations (III) in the international conferences and overseas institutions in the past year or so.

英文關鍵詞： plasmonic nanomaterial, metal nanoparticle, optical property, electromagnetic simulation

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）電漿子奈米材料之電磁理論與模擬研究

Electromagnetic theory and simulation of plasmonic nano-materials

計畫類別：■個別型計畫　□整合型計畫
計畫編號：NSC　100－2112－M－004－002
執行期間：　100 年 8 月 1 日至　101 年 10 月 31 日

執行機構及系所：國立政治大學應用物理研究所

計畫主持人：郭光宇
計畫參與人員：鄭為晉、詹勳奇(碩士班學生），陳志寰（專任助理)，
董人銓(博士後研究員）

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

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
□國際合作研究計畫國外研究報告

處理方式：除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

中　華　民　國　102 年 1 月 9 日

附件二

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）

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）

The principal purpose of this proposal is to understand the origin and mechanism of the exciting surface plasmon-related phenomena in a range of metal nanomaterials. This has been be achieved primarily by performing extensive numerical electromagnetic simulations. In the past year, we have exploited several complementary frequency-domain methods [e.g., the discrete dipole approximation (DDA) and finite-element, methods] as well as the time-domain method [i.e., finite-difference time domain (FDTD) method)] to investigate the physical properties of a number of novel metamaterials sytems. Indeed, our fascinating and important results have been published in 12 papers in international journals [e.g., very prestigious physics journal Phys. Rev. Lett. (10) and very prestigious nano-science journal Nano Letters (12)] (see the enclosed publication list below) since Aug. 1, 2011. We have also interacted and collaborated actively with many experimental and theoretical groups at home and abroad.

Some research highlights are described in more details below (I). Also enclosed in this report are the list of publications (II) and the list of invited presentations (III) in the international conferences and overseas institutions in the past year or so.

The Final Report on the National Science Council Research Grant

(NSC-100-2112-M-004-002**)**

Guang-Yu Guo (郭光宇),

Graduate Institute of Applied Physics, National Chengchi University

The principal purpose of this proposal is to understand the origin and mechanism of the exciting surface plasmon-related phenomena in a range of metal nanomaterials. This has been be achieved primarily by performing extensive numerical electromagnetic simulations. In the past year, we have exploited several complementary frequency-domain methods [e.g., the discrete dipole approximation (DDA) and finite-element, methods] as well as the time-domain method [i.e., finite-difference time domain (FDTD) method)] to investigate the physical properties of a number of novel metamaterials sytems. Indeed, our fascinating and important results have been published in 12 papers in international journals [e.g., very prestigious physics journal Phys. Rev. Lett. (10) and very prestigious nano-science journal Nano Letters (12)] (see the enclosed publication list below) since Aug. 1, 2011. We have also interacted and collaborated actively with many experimental and theoretical groups at home and abroad.

Some research highlights are described in more details below (I). Also enclosed in this report are the list of publications (II) and the list of invited presentations (III) in the international conferences and overseas institutions in the past year or so.

I. Research highlights

1. *Coherent perfect nanoabsorbers based on negative refraction:*

Recently, a fascinating concept of coherent perfect absorbers (CPAs) has been suggested. In some sense this concept is an inverse to the concept of lasing. This conception was demonstrated experimentally by the example of a symmetric Fabry-Perot cavity with small losses which was symmetrically irradiated by 2 coherent plane waves (see Fig. 1). It was shown that under certain conditions, all the energy of incoming waves is fully absorbed by the dielectric (silicon) slab. As a result, the radiation from the system disappears for some parameters. This situation indeed is reciprocal to the case of lasing, where for high enough pumping the coherent radiation appears. More complicated examples of CPA with plane waves were considered.

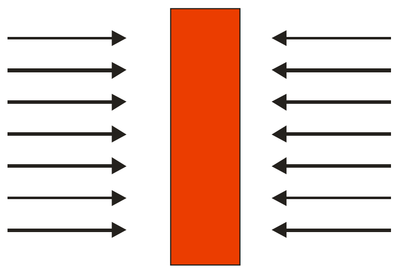

Fig. 1. Schematic diagram of a plane wave coherent perfect absorber.

Despite generic nature of this concept, its application to more complicated geometries is a nontrivial task. In particular, since now the control of radiation of atoms and molecules with nanoparticles and metamaterials becomes very important, it is desirable to have an effective nanoabsorber of electromagnetic fields from a single atom or molecule. First of all, one may have a complicated spatial structure of light field. For example, the emission pattern of an atom would correspond to spherically divergent beams rather than plane waves. Moreover, many applications nowadays are related with making use of metamaterials for the control of light at the nanoscale.

In the present work, we propose a concept of coherent perfect nanoabsorbers (CPNAs) using a slab made of double negative (DNG) metamaterial, that is, the metamaterial with negative refractive index. Nowadays, slabs with negative refraction are widely used for many applications such as perfect lensing and cloaking of small objects. Our concept is based on recently discovered focusing properties of a system of sources and sinks near a slab with negative refraction, where it was shown that if two sources and one sink were put at the ray intersection points, all the energy from the sources would go to the point sink. In this paper we propose to use a real nanoparticle instead of the hypothetic sink used. The operation scheme of our CPNA is shown schematically in Fig. 2. The device shown in Fig. 2 would allow absorbing all the energy from the 2 sources emitted in the direction towards the negative refraction slab by a nanoparticle placed inside it.

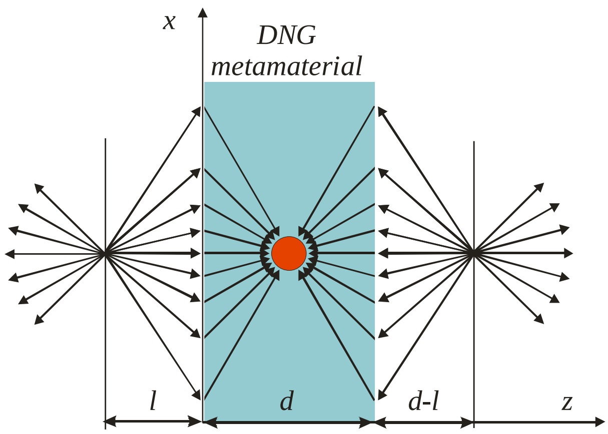

Fig. 2. Schematic diagram of a coherent perfect nanoabsorber for the divergent beams. All the energy from the 2 point sources is absorbed by the nanoparticle (red circle), placed inside the negative refraction slab.

It should be emphasized that within the geometry of Fig. 2, only half of the radiated energy is going towards the slab and then absorbed. However, it is a trivial task to slightly modify this system by adding perfect magnetic mirrors just behind the *x*-polarized dipoles. This would result in doubling of the radiated energy going to the slab and then absorbed. For *z*-oriented dipoles, one should use perfect electric mirrors to absorb all the radiated energy. For simplicity, we will consider here only the systems without mirrors.

2. *High-efficiency broadband anomalous reflection by gradient meta-surfaces:*

As is well known in optics community, light reflections/refractions at an interface between two different homogeneous media satisfy the famous Snell's law. Beginning from 2011, rather unexpectedly, a series of works (Capasso's group Science 2011, Shavalev's group Science 2012) have shown that Snell's law can be generalized when one of the media is replaced by a carefully designed inhomogeneous meta-material which provides an additional k vector to the momentum conservation. Different from the former works to convert incident propagating waves (PWs) to anomalous reflected PWs, we further extended this idea to show that such a meta-surface can convert PWs to surface waves with 100% efficiency. These works are certainly of great importance to the optics community. Our system behaves as an efficient bridge between far field and near field and hence is highly desired for the development of plasmonics.

Despite of the great successes already achieved for the above introduced gradient mate-surfaces, these works still suffer some limitations. For example, available meta-surfaces so far designed by these groups only work in the infra-red (IR) and microwave regimes, and the generalized Snell's law has not yet been tested in visible regime, which is certainly more challenging and interesting. Also, previously fabricated IR meta-surfaces (Capasso's group & Shavalev's group) support not only anomalous reflections/refractions, but also support normal ones simultaneously, so that the desired effects do not exhibit high efficiency (~20% or so). Very recently, we theoretically and experimentally demonstrate a carefully designed gradient meta-surface that supports high-efficiency anomalous reflections governed by the generalized Snell's law at ~850nm wavelength. The anomalous reflected wave can be either non-specular propagating waves or surface waves determined by the incident angle of the input beams. Compared to previously fabricated gradient meta-surfaces in infra-red wavelength regime (Capasso's group & Shavalev's group), our samples work at a shorter wavelength regime with a broad bandwidth (700-900nm). The conversion efficiency to the anomalous reflection mode is up to about 80% and the polarization of the anomalous reflected beams keeps unchanged.

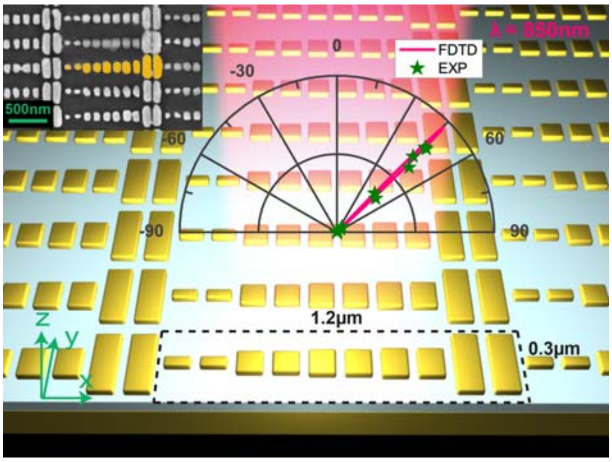

Figure 3. Geometry of the metasurface and anomalous reflection demonstration.

II. Publication list:

Twelve (12) high quality papers have been published in international SCI journals since Aug. 1, 2011, including one paper in the prestigious physics journal Physical Review Letters [10] and one paper in the prestigious nano-science journal Nano Letters [12].

[1] J.-H. Li, J.-D. Chai, G. Y. Guo and M. Hayashi,
The quantified NTO analysis for the electronic excitations of molecular many-body systems
Chem. Phys. Lett. 514, 362 (Oct., 2011) [SCI].

[2] H. C. Hsueh, G. Y. Guo, and S. G. Louie
Excitonic effects in the optical properties of a SiC sheet and nanotubes,
Physical. Review B 84, 085404 (Aug., 2011) [SCI]

[3] H.-R. Fuh and G. Y. Guo
Intrinsic anomalous Hall effect in nickel: A GGA + U study,
Physical Review B 84, 144427 (Oct., 2011) (IF:3.5)

[4] T.-W. Chen, Z.-R. Xiao, D.-W. Chiou, and G. Y. Guo,

High Chern number quantum anomalous Hall phases in graphene ribbons with Haldane orbital coupling, Physical. Review B 84, 165453 (Oct., 2011) (IF:3.5)

[5] J.-H. Li, J.-D. Chai, G. Y. Guo, M. Hayashi
Significant role of the DNA backbone in mediating the transition origin of electronic excitations of B-DNA - implication from long range corrected TDDFT and quantified NTO analysis
PHYSICAL CHEMISTRY CHEMICAL PHYSICS 14 (2012) 9092

[6] C. C. Chen, C. T. Hsiao, S. L. Sun, K. Y. Yang, P. C. Wu, W. T. Chen, Y. H. Tang, Y. F. Chau, E. Plum, G. Y. Guo, N. I. Zheludev, D. P. Tsai, *Fabrication of three dimensional split ring resonators by stress-driven assembly method,* OPTICS EXPRESS 20, 9415-9420 (2012)

[7] V. Klimov, S. L. Sun, G. Y. Guo,
Coherent perfect nanoabsorbers based on negative refraction
OPTICS EXPRESS 20 , 13071-13081 (2012)

[8] Y.-F. Hsu, T.-W. Chiang, G. Y. Guo, S. F. Lee, J.-J. Liang
Effect of Transport-Induced Charge Inhomogeneity on Point-Contact Andreev Reflection Spectra at Ferromagnet-Superconductor Interfaces, J. Phys. Soc. Jpn. 81 (2012) 084701

[9] J.-C. Tung, H.-R. Fuh and G. Y. Guo
Anomalous and spin Hall effects in hcp cobalt from GGA + U calculations
Physical Review B 86, 024435 (2012)

[10] P. He, L. Ma, Z. Shi, G. Y. Guo, J.-C. Zheng, Y. Xin, and S. M. Zhou
Chemical Composition Tuning of the Anomalous Hall Effect in Isoelectronic L10 FePd1-xPtx Alloy Films
Physical Review Letters 109, 066402 (2012)

[11] S. W. Chen, S. C. Huang, G. Y. Guo, S. Chiang, J. M. Lee, S. A. Chen, S. C. Haw, K. T. Lu and J. M. Chen, *A combined first principle calculations and experimental study on the spin-polarized band structure of Co-doped* $PbPdO_2$, Appl. Phys. Lett. 101, 222104 (2012)

[12] S. L. Sun, K.-Y. Yang, C.-M. Wang, T. K. Juan, W. T. Chen, C. Y. Liao, Q. He, S. Y. Xiao, W. T. Kung, G. Y. Guo, L. Zhou and D. P. Tsai,
High-efficiency broadband anomalous reflection by gradient meta-surfaces,
Nano Letters 12, 6223 (2012)

III. Invited talks and lectures:

[1] Invited lecture titled “Ab Initio Studies of Electronic Structure, Magnetism and Ferroelectricity in $BiMnO_3$ and $Li(Na)Cu_2O_2$”, in the Advanced School on Modeling Complex Oxide, S. N. Bose Center, Kolkata, India, April 9-13, 2012

[2] Invited talk titled “Ab Initio and Quantum Monte Carlo Studies of Spin Hall Effect in Metals”, in Psik-k Research Conference on Computational Oxide Spintronics, Holmes Chapel, UK, May 6-10, 2012

[3] Invited Seminar titled “Physics of Spin Hall Effect”, in Physics Department, University of York, UK, May 11, 2012

[4] Invited seminar titled “Optical Magnetic Meta-materials and Coherent Perfect Nanoabsorbers: Design, Fabrication and Properties”, in P. N. Lebedev Physical Institute, Russian Academy of Sciences, Moscow, Russia, July 4, 2012

附件四

國科會補助專題研究計畫項下出席國際學術會議心得報告

日期：___年___月___日

計畫編號	NSC 100－2112－M－004－002		
計畫名稱	電漿子奈米材料之電磁理論與模擬研究		
出國人員姓名	郭光宇	服務機構及職稱	國立政治大學應用物理研究所
會議時間	2012年5月6日至2012年5月10日	會議地點	英國 Holmes Chapel
會議名稱	(中文) (英文)Psi-K Research Conference on Computational Oxide Spintronics		
發表論文題目	(中文) (英文) Ab Initio and Quantum Monte Carlso Studies of Spin Hall Effect in Metals		

一、參加會議經過

二、與會心得

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

六、其他

參加 Psi-K Research Conference on Computational Oxide Spintronics 國際會議(英國)並順道訪問英國 Salford 和 York 大學之報告(May 10-13, 2012)

政治大學應用物理研究所 郭光宇

The Conference: A broad variety of physical properties make transition-metal oxides (TMO) a unique class in modern materials science, where a rich and exciting fundamental physics is nicely joined to a huge potential for technological spintronic applications whose harvesting relies on fundamental progress on theoretical physics, computational methodology and tools. Moreover, the many competing energy scales in TMO make their response to external stimuli a vast playground for colossal cross-coupled effects to emerge and at the same time a challenge for a computational description. Finally, novel TMO functionalities have recently been shown to be induced or tuned or switched by the formation of heterostructures or at the nanoscale. A consensus is therefore emerging: transition metal oxides will constitute basic materials for a novel generation of spintronic devices. Understanding and exploiting their properties is therefore one of the key challenges in current computational material science.

Complexity in functional oxides poses a set of challenges from the modeling point of view, calling for an accurate treatment of correlated 3d- or 4f-electrons and excited states as well as for a careful description of the delicate coupling between electronic degrees of freedom to structural distortions and crystal symmetries. Indeed, what is required is an arsenal of computational tools, ranging from methods able to study complex structures, over various degrees of correlation phenomena, spectroscopy, functional aspects, interfaces, defects, coupling of electric (magnetic) fields to magnetic (electric) polarization and to non-equilibrium quantum transport. Moreover, the manipulation of spin-transport through junctions based on oxides could be further developed as well as transport properties controlled by spin-orbit coupling.

While many groups are actively involved in research focused on oxides in Europe, USA and Asia, there are few opportunities for workshops focused on “oxides modeling”. Therefore, this conference was aimed at filling this gap by organizing a research conference, where discussions (coordinated by world-wide renowed “discussion leaders”) should be very lively and where presentations should not only consist of general talks targeted to a broad audience, but should also illustrate advanced computational methodologies or progresses in implementations, including technical aspects. It was planned to bring together different communities: density functional theorists, many-body physicists, experts on theory of magnetism, of ferroelectricity, of transport, etc. A few world-leading scientists (Agnes Barthelemy of France, Rainer Waser of Germany; David Vanderbilt of USA; Yoshinori Tokura of Japan) were invited to give plenary talks.

The trip: I left Taiwan Taoyuan International Airport in the morning of May 3 at 9:00 am via Taiwan Eva Airline, and after a brief stopover at Bankok Airport in Thailand, arrived in the London Heathrow Airport at 19:15 pm (May 3). I then took a British Airway (BA) flight from London Heathrow Airport at 21:30 pm to arrive in the Manchester Airport at 22:30 pm. I finally took a train from Manchester Airport to Manchester Piccadilly Station and then a taxi from the Rail Station to arrive at the Hotel almost mid-night. I then spent the next two day (Thursday and Friday) in Salford University. I went to Holmes Chapel in the

Sunday morning (May 6) for the Psik-k Research Conference which was the main purpose of my trip to the UK this time. Left Holmes Chapel right after the Conference at 12:30 noon on Thursday, May 10, and arrived in York at about 16:00 pm in the same day. I then spent next one and half days (Friday and Saturday) in the University of York. Finally, I left York in the afternoon of Saturday (May 12) by the fast East Coast Train to London, and it took only about 2 hours. After that, I took a London Underground train to London Heathrow Airpot. I left London Heathrow at 21:35 pm on May 12, and arrived in Taoyuan International Airport in the evening of May 13 at 21:30. It was a rather long but smooth, very stimulating and fruitful trip.

The \activities: (1) In Salford University from May 4 to May 5: I gave a seminar titlted "Physics of Spin Hall effect" (see the abstract enclosed below) on Friday from 13:00 to 14:00 in School of Computing, Science and Engineering. Before my talk, I discussed with one of PhD students of Dr. Tiehan Shen in the Materials and Physics Division the possible dichroism in the optical spectra from the metallic nano-objects grown on the Si substrate. We have also been study theoretically this kind of electromagnetic metamaterials. Dr. Shen's group has been work on experimental synthesis and characterization of these metamaterials, and therefore, the purpose of this discussion is how to write a joint paper on this topic. After my talk, I went to talk to Prof. Ian Morrison (also an electronic structure theorist) on computational studies of hygroden energy materials such as graphene-related structures. In particular, both Salford U. and Manchester U., where the graphene was first discovered and studied, are the same city. After that, I visited several laboratories. On the Saturday (May 5), Dr. Shen (my host) and I had some extensive discussions on our ongoing joint research projects especially on magnetic and spintronic materials, as well as plasmonic metamaterials. Indeed, we have been preparing a joint manuscript titled "Effects of spin-resolved density of states on optically excited polarized electron injection over Ni/GaAs Schottky barrier", to combine my electronic structure results on bulk Ni with his spin-dependent photoconductivity measurements.

(2) In the conference: I will leave Manchester for Holmes Chapel where the Psi-K Research Conference will be held, on July 6.

I will leave Holmes Chapel right after the Psi-K Research Conference for York at 13:00 on May 10, via Trains. Therefore,

(3) In the York Univesity: On May 11 and 12, I spent one and half day in the School of Physics and Astronomy. In the morning of Friday, May 11, two PhD students from Dr. Irene D'Amico and Prof. Roy Chantrell's groups, came to talk to me about the theoretical work on calculating the damping coefficient in the Landau-Liftshift-Gilbert equation for the magnetic materials. Prof. Roy Chantrell has been in tough and collaboration with Prof. Ching-Ray Chang (National Taiwan University) and myself for some time. In fact, one of the two students stayed in NTU for about one month last year (2011). I then went to talk to Prof. Rex Godby, a condensed matter many-body theorist who I have known since when I was a PhD student in the Cambridege University. My seminar on "Physics of Spin Hall Effect" (see the attached abstract below) is scheduled to start at 14:00, and finished at 15:30, apparently that it went on so well that extra time was given. After the seminar, I went to join the faculty afternoon tea break, chatting to several faculty members there. On the morning of Saturday, May 12, Prof. Jun Yuan (my host) showed me several laboratories, and afterwards, we had an extensive discussion especially the properties of electron and photon beams with orbital angular momenta, and also on electronic materials.

In short, my trip to the UK was really a very stimulating and fruitful one. I learned many things and also made several new friends in this trip. Therefore, I would like to thank the National Science Council for supporting this trip to the UK.

在 Salford 和 York 大學的學術演講 (Seminar)（May 4和 May 11）的摘要:

Physics of Spin Hall Effect

Guang-Yu Guo[1,2*]

[1]*Graduate Institute of Applied Physics, National Chengchi University, Taipei 116, Taiwan*

[2]*Department of Physics, National Taiwan University, Taipei 106, Taiwan*

**E-mail: gyguo@phys.ntu.edu.tw*

Spin Hall effect (SHE) refers to the generation of transverse spin current in a solid by an electric field. Spin current generation is an important issue in the emerging spintronics technology. Thus, SHE has recently attracted considerable interest both theoretically and experimentally since the theoretical proposals of the intrinsic SHE [1-2]. In this talk, I will first give an introduction to SHE, and then describe *ab initio* calculation approaches to the various issues in the field of SHE, in particular, Berry phase theory and *ab initio* relativistic band structure method [3,4]. This will be followed by a review on our recent relativistic band theoretical studies on the intrinsic SHE in Pt, Al [4], Pd, Au [5] and Mo. In particular, our *ab initio* calculations revealed that the resonant contribution from the spin-orbit splitting of the doubly degenerated *d* bands near the Fermi level gives rise to a large intrinsic spin Hall conductivity in Pt and Pd.

Furthermore, our electronic structure calculations for various transition metal impurities in gold indicated possible orbital-dependent Kondo effect in Fe impurity in Au [6]. Thus, the gigantic SHE observed recently in FePt/Au system [7] was attributed to resonant skew scattering due to multi-orbital Kondo effect [6]. Our estimated spin Hall angle is about 0.1, in agreement with the measured value [7]. Indeed, our subsequent quantum Monte Carlo simulations for a realistic three-orbital Anderson impurity model demonstrated two Kondo temperatures in Fe in Au: one very low Kondo temperature for Fe d_{eg}-states and the other high Kondo temperature for Fe t_{2g}-states [8]. It was also found that the spin-orbit interaction and hence the SHE is strongly renormalized by the quantum spin fluctuation. This explains why the gigantic SHE in Au with Fe impurities was observed in recent experiments, while it is not visible in the anomalous Hall effect. Moreover, latest experiments on Au films with well controlled Fe impurity concentrations confirmed that the spin Hall angle is about 0.07 and independent of Fe impurity concentration [9], thereby indicating the extrinsic nature of the SHE observed in FePt/Au systems.

The speaker thanks Naoto Nagaosa, Bo Gu, Sadamichi Maekawa, Tsung-Wei Chen, Shuichi Murakami, and Qian Niu for stimulating discussions and collaborations. He also thanks the National Science Council of Taiwan for financial supports.

[1] S. Murakami, N. Nagaosa, and S.-C. Zhang, Science **301**, 1348 (2003); [2] J. Sinova *et al.*, Phys. Rev. Lett. **92**, 126603 (2004); [3] G. Y. Guo, Y. Yao and Q. Niu, Phys. Rev. Lett. **94**, 226601 (2005); [4] G. Y. Guo, S. Murakami, T. W. Chen, and N. Nagaosa, Phys. Rev. Lett. **100**, 096401 (2008); [5] G. Y. Guo, J. Appl. Phys. 105, 07C701 (2009) ; [6] G. Y. Guo, S. Maekawa, and N. Nagaosa, Phys. Rev. Lett. **102**, 036401 (2009); [7] T. Seki *et al.*, Nature Mater. **7**, 125 (2008) ; [8] B. Gu, J.-Y. Gan, N. Bulut, T. Ziman, G. Y. Guo, N. Nagaosa and S. Maekawa, Phys. Rev. Lett. 105, 086401 (2010).

Science & Technology Facilities Council

Event Booking System

Psi-k Research Conference on "Computational Oxide Spintronics" - Agenda

Return to event

Agenda Day 1 - 07/05/2012

0900 - 1000
Plenary - Barthelemy
Agnes Barthélémy - Unité Mixte de Physique CNRS/thales
1000 - 1100
Oxide-based Interfaces - Ghosez
TBC
1100 - 1130
Coffee
Shirley Miller - Science and Technology Facilities Council
1130 - 1230
Oxide-based Interfaces - Pentcheva
Rossitza Pentcheva - University of Munich
1230 - 1330
Lunch
1330 - 1430
Free time for discussion
1430 - 1530
Oxide Tunnel Junctions - Tsymbal
Evgeny Tsymbal - University of Nebraska-Lincoln
abstract-tsymbal.doc
1530 - 1630
First-principles design of magnetic oxidic surfaces and interfaces
Arthur Ernst - MPI Halle
aernst-abstracts.doc
1630 - 1700
Coffee
1700 - 2000
Poster Session
2000 - 2200
Dinner

Agenda Day 2 - 08/05/2012

0900 - 1000
Plenary - Vanderbilt
David Vanderbilt - Rutgers University
1000 - 1100
Topological transport and Berry phases - Souza
Ivo Souza - university of the Basque Country
1130 - 1230
Topological transport and Berry phases -

Guang-Yu Guo - National Taiwan University, Department of Physics
1230 - 1330
Lunch
1330 - 1430
Beyond LDA functionals - Kresse
1430 - 1530
Beyond LDA functionals - Rinke
Patrick Rinke - Fritz-Haber-Institut der MPG
1530 - 1600
Coffee
1600 - 1700
DMFT and Electronic Correlations - Biermann
Silke Biermann - Ecole Polytechnique
1700 - 1800
DMFT and Electronic Correlations - Liechtenstein
1800 - 2000
Free time for discussion

Agenda Day 3 - 09/05/2012

0900 - 1000
Plenary - Waser
1000 - 1100
Defects in oxides and high-k materials - Sanyal
1100 - 1130
Coffee
1130 - 1230
Defects in oxides and high-k materials - TBA
TBC
1230 - 1330
Lunch
1330 - 1430
Superconductivity and Interplay with Magnetism - Singh
David Singh - Oak Ridge National Laboratory
1430 - 1530
Superconductivity and Interplay with Magnetism - Antropov
1530 - 1930
Free time and Social Dinner (coach leaves 1930 for Swettenham Arms)
Visit Website
1900 - 2300
Coach Leaves Cranage Hall
Shirley Miller - Science and Technology Facilities Council

Agenda Day 4 - 10/05/2012

0900 - 1000
Plenary - Tokura
1000 - 1100
Multiferroics and magnetoelectrics - Ederer
Claude Ederer - ETH Zürich
1100 - 1130
Coffee
1130 - 1230
Multiferroics and magnetoelectrics - Fennie
Craig Fennie - Cornell University
1230 - 1330
Lunch

Return to event

The Psi-K Research Conference on Computational Oxide Spintronics 邀請演講 (Invited Talk)摘要 (May 9, Cranage Hall, Holmes Chapel, UK):

Ab Initio and Quantum Monte Carlo Studies of Spin Hall Effect in Metals

Guang-Yu Guo[1,2*]

[1]*Graduate Institute of Applied Physics, National Chengchi University, Taipei 11605, Taiwan* [2]*Department of Physics, National Taiwan University, Taipei 10617, Taiwan*

**E-mail: gyguo@phys.ntu.edu.tw*

Type of Contribution: an invited talk (please indicate if you prefer oral or poster)

Spin Hall effect (SHE) refers to the generation of transverse spin current in a solid by an electric field. Spin current generation is an important issue in the emerging spintronics technology. Thus, SHE has recently attracted considerable interest both theoretically and experimentally since the theoretical proposals of the intrinsic SHE in 2003. In this talk, I will first give an introduction to SHE. I will then describe *ab initio* calculation approaches to the various issues in the field of SHE, in particular, Berry phase theory and *ab initio* relativistic band structure methods for studying intrinsic SHE [1,2]. This will be followed by a review on our recent *ab initio* studies on the intrinsic SHE in Pt, Al[2], Pd, Au [3] and Mo. In particular, our *ab initio* calculations revealed that the resonant contribution from the spin-orbit splitting of the doubly degenerated *d* bands near the Fermi level gives rise to a large intrinsic spin Hall conductivity in Pt and Pd. These predictions agree well with recent experiments [4,5]. Furthermore, our *ab initio* electronic structure calculations for various transition metal impurities in gold indicated possible orbital-dependent Kondo effect in Fe impurity in Au [6]. Thus, the gigantic spin Hall effect observed recently in FePt/Au system [7] was attributed to resonant skew scattering due to multi-orbital Kondo effect [6]. Our estimated spin Hall angle is about 0.1, in agreement with the measured value [7]. This explains why the gigantic SHE in Au with Fe impurities was observed in recent experiments, while it is not visible in the anomalous Hall effect. Indeed, our subsequent quantum Monte Carlo simulations for a realistic three-orbital Anderson impurity model demonstrated two Kondo temperatures in Fe in Au: one very low Kondo temperature for Fe d_{eg}-states (a few Ks) and the other high Kondo temperature for Fe t_{2g}-states (above room temperature) [8], and the spin Hall effect to be strongly enhanced by quantum spin fluctuation in the high temperature Kondo regime. Furthermore, latest experiments on Au films with well controlled Fe impurity concentrations confirmed that the spin Hall angle is about 0.07 and independent of Fe impurity concentration [9], thereby indicating the extrinsic nature of the SHE observed in FePt/Au systems.

The speaker thanks Naoto Nagaosa, Bo Gu, Sadamichi Maekawa, Tsung-Wei Chen, Shuichi Murakami, Qian Niu for stimulating discussions and collaborations. He also thanks the National Science Council of Taiwan for financial supports.

[1] G. Y. Guo *et al.*, Phys. Rev. Lett. **94**, 226601 (2005); [2] G. Y. Guo *et al.*, Phys. Rev. Lett.

附件四

國科會補助專題研究計畫項下出席國際學術會議心得報告

日期：___年___月___日

計畫編號	NSC 100－2112－M－004－002		
計畫名稱	電漿子奈米材料之電磁理論與模擬研究		
出國人員姓名	董人銓	服務機構及職稱	國立政治大學應用物理研究所
會議時間	2012年10月14日至2012年10月18日	會議地點	日本神戶
會議名稱	(中文) 2012 計算物理年會 (英文) Conference on Computational Physics 2012		
發表論文題目	(中文)利用第一原理計算鈷類別的Heusler合金的自旋與異常霍爾電導 (英文) Spin and Anomalous Hall Conductivities in Co-based Heusler Alloys: A First-principle Study		

一、參加會議經過

今年的CCP2012在日本神戶舉辦，舉辦的地點在“K computer”附近。 第一天我中午到大阪關西機場，下午就順利到達會議會場並完成註冊。會議第一天2012/10/15：今天會議早上一開始就講我不熟的Quantum Monte Carlo Simulation. 其實今天整天大部份都這類型的演講，在台灣這個領域還不算蓬勃發展，因為我們沒有合適的電腦來作這類型的計算。會議第二天 2012/10/16：早上第一場講Laser simulation, 與會人士問了一個非常有趣的問題 ”用電腦模擬一次Laser pulse, 需要的能量, 跟真正用雷射作一次實驗, 兩者相差多少？”緊接著就是 Silicon Cluster的分子動力學模擬與amino acids, protein folding之類的模擬。Break之後緊接著，大師出現了，Stefan Blugel !他講了一個非常有趣的論點： 我們通常使用PBE correlation function 作計算，而這樣的計算通常比起LDA要多花100倍的時間(complexity)，或許你會想說，沒關係，我們有K computer，聽到這裡大家都笑了。大師竟然也有風趣的一面。接下來則是今年年輕研究學者的演講，他從古典的蒙地卡羅方法一路講到Quantum Information, Quantum Monte Carlo。他主要是討論Quantum Spin Liquid的議題。

從今天下午開始，就有 DFT 方面的議題了，我竟然碰到了 Prof. Ishibashi, 真是太巧了。第一個 talk, 提到了ＤＦＴ不能正確的算出 VO_2 的能帶，讓我感到好奇。我回台灣以後要算看看，接下來的演講多是跟電池有關的議題。我不是很懂這個議題，不過看起來很有趣的樣子。今天最後的 poster session 換我上去了，因為今年沒有磁性相關的議題，所以我雖然報名要給個口頭演講，但還是被移到 poster session. Poster 我被排在第 101 號，有大約 6 位與會者對我的研究有興趣，跑來與我進行學術討論，還有兩位是因為郭光宇所長在日本 JIAST 認識的研究學者來與我聊天。這天的 poster 種類從天文到氣候預測都涵蓋了，可以說電腦模擬這個領域已經滲透到各個方面了。

會議第三天 2012/10/17：今天一早就講到日本的 K computer 的計畫始末，事實上昨天 Blugel 也提到他在德國使用的 IBM Blue Gene 的計算能力只有 K computer 的 1/30 ，日在這方面真是下了很多的心力。這裡有一個小插曲，就是講者的電腦有問題，所以一直不能開始。他不斷的向與會人士道歉，大會也緊急提供一台筆電供他使用，怪了，不是應該要是先檢查好的嗎？接下來也是介紹電腦與半導體進展的論文。這兩場結束後，接下來的演講是有關 Lattice QCD 的，原來，這領域需要更強猛的電腦阿～隨便一個模擬，如果電腦不夠力，都要花上幾百幾千年的，太嚇人了。緊接著，是關於大尺度的蒙地卡羅模擬的方法，尺度非常的大，所以一定要有特別的方法才能做到。聽完這場後，早上的會議就結束了。

下午的會議，我看了半天的 program，最後我決定參加跟軟體開發有關的 session, 因為其他的感覺都跟我會的差很多。這個議程果然，參與的人並不多，然後，報告者又搞不定他的電腦與投影機接續的問題了，怎麼會這樣呢？最後他放棄了他那台筆電，然後請下一個講者先上場。又晚了 30 分鐘才開始今天下午的議程。代替上場的講者從 BERKELEY 來的，他們發展一個叫做 Chombo 的 open source 軟體，這個軟體是用來求解偏微分方程式的：Software for Adaptive Solutions of Partial Differential Equations ，接下來是來自東京大學的，他們發展一個叫做ＡＬＰＳ的軟體來計算強關聯系統。最後一場是來自ＬＳＵ的 Frank Loffler，他講的是 Einstein Tools Kit：純天文模擬的軟體。

會議第四天 2012/10/18：今天，竟然用到了同步口譯。大會請來了朝日新聞的 Editor 來給大家一些，市民關於計算物理這個領域在一般人心中的看法，以及一般市民對計算物理這個領域的期望。我想，大概是這幾年日本花很多錢在建置計算設施上，像是 K computer，還有 Earth Simulator 等等。非常值得注意的是，日本最早的計算物理前沿計畫竟然是 97 年才開始的，才 15 年的時間，日本已經進步到這個程度了，而我們連個像樣的計算設施都沒有。不過話說回來，日本富士建造 K computer 花了 112 billion，然而現在的第一名美國的 Sequoia 則花不到 20 billion. 怎麼會這樣呢 ? 我想，台灣沒這能力也不需要去競爭第一名或者花那麼多錢，但是充足的計算資源是我們深切需要的。這個演講完後的討論非常的熱烈，特別是 電腦計算能不能稱為第三科學？ 電腦計算能不能 “解決“ 像是人類學，地震，颱風等等議題？ 尤其是現在的超級電腦，也許 50 年後效能跟當時的個人電腦相同，那為什麼現在要花這麼多錢？

雖然是最後一天，但是議程依然是排到下午四點，這樣的安排真是太晚了。第一場講到 Density-matrix functional theory, 接下來是來自韓國的學者講 Strain-dependent magnetism 這個題目跟我最近在研究的好像有關。首先作者提到了單個 Cs 長在 Graphene 上的情形，然後更進一步再看看過渡金屬長在 graphene 上的情況，這我以為應該是很多年前的研究了，沒想到竟然是 2011 年發表的。接下來講到同樣的情況在 BN 上，那我想也可以考慮在 SiC 上吧。這裡有一個地方我覺得比較難的是，她有考慮到 Vacancy 造成的影響，還有考慮加電場下的行為。接下來的講者，很有趣的，竟然用 OPENMX 加 COMSOL 去算 GNR 在有缺陷(圓形，三角形或正方形)下的光學行為。不過他這個計算不是週期性的，所以可能需要某種特別的方法。接下來的講者，利用 TDDFT

研究原子碰撞的行為。大體上就是系統的位能計算方式與一般的 DFT 甚至 TDDFT 不同，所以需要用到 K computer。最後一個講者，與前前一個講者，都是來 JIAST 拿學位的國際學生。我想，有好的研究環境與研究資源，自然會吸引各國的年輕學子來。聽完這場以後，時間也來到下午四點，緊接著就是大會閉幕儀式了，我也順利結束這場會議。

二、與會心得

這次參加會議，看到了電腦計算的新進展。許多與會者的研究，在台灣幾乎都不可能達成，即使研究人員有心，也沒有辦法在台灣完成，只能靠國際交流。不過，透過參與這類型的國際會議，對我的研究見解，也有所助益。

三、發表論文全文或摘要

Spin and Anomalous Hall Conductivities in Co-based HeuslerAlloys: A First-principle Study

Jen-Chuan Tung[1] **and Guang-Yu Guo**[1,2]

[1]Graduate Institute of Applied Physics, National Chengchi University, Taipei 11605, Taiwan

[2]Department of Physics and Center for Theoretical Sciences, National Taiwan University, Taipei 10617, Taiwan

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Abstract. Spin-dependent electronic transports have recently attracted muchattention becausethey not only are interesting from the viewpoint of fundamental physics, but also have useful applications. Both the anomalous and spin Hall effect are one of the spin-related transport phenomena and hence haveconsiderable interests in recent years. Many of the full Heusler alloys, especially Co-based Heusler compounds (denoted as Co_2XZ) are predicted to be half-metallic ferromagnets and hence have potential applications in spintronics. Therefore, we have recently calculated the intrinsic spin Hall conductivity (SHC) and anomalous Hall conductivity (AHC) as well as other physical properties of someCo-based full Heusler alloys by using the density functional theory with generalized gradient approximation. The accurate all-electron full-potential linearized augmented wave method is used. Firstly, we find that the calculated AHC for Co_2CrAl, Co_2MnSi, and Co_2MnSn are in good agreement with recent experiment, suggesting the intrinsic origin of the anomalous Hall effect in these compounds. Secondly, we estimate the spin polarization (P^H)of Hall current using the calculated AHC and SHC. Remarkably, we find that the spin polarization (P^H) of the Hall current is 100% for all the compounds considered except Co_2CrGa.

四、建議

五、攜回資料名稱及內容

六、其他

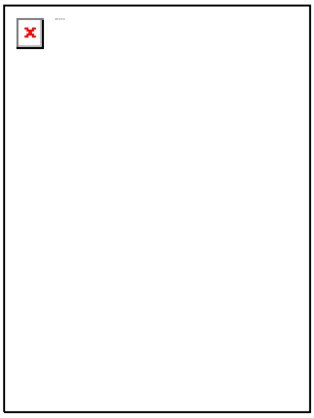
附件五

國科會補助專題研究計畫出席國際學術會議心得報告

日期：101 年 10 月 29 日

計畫編號	NSC 100-2112-M-004-002		
計畫名稱	電漿子奈米材料之電磁理論與模擬研究		
出國人員姓名	陳志寰	服務機構及職稱	國立政治大學應用物理所 研究助理
會議時間	01 年 10 月 14 日至 01 年 10 月 18 日	會議地點	日本 神戶, Nichii Gakkan Conference Center
會議名稱	(中文) 2012 計算機物理年會 (英文) Conference on Computational Physics 2012		
發表題目	(中文) 利用第一原理計算 3d 過渡金屬鋸齒狀結構原子線的自旋螺旋波 (英文) Spin-spiral waves in zigzag 3d transition metal atomic chains from first principle calculations		

一、參加會議經過



這次會議為期五天 2012 年 10 月 14 日到 18 日，總數有 323 個會議演講、parallel sections 演講與海報論文，會議地點在神戶市人造島 Nichii Gakkan conference center，附近有 K computer、神戶大學與兵庫大學。剛到神戶第一天(10/14)在會議註冊前在神戶三宮駛附近東橫 inn 飯店下榻，遇到在清大的學弟邱昶偉，他剛好是到日本兵庫縣姬路市附近的 SPring-8 同步輻射中心做實驗，然後要回台灣途中來神戶參觀跟交換他們的研究成果與心得，有股他鄉遇故知的感覺，所以在簡單放完行李就出門前往會場註冊，第一天晚上也在神戶三宮車站附近逛了商店街、百貨公司，晚餐簡單吃了百貨公司買回來的平價打折握壽司，晚上也早點休息為了隔天會議早起。

會議議程第一天十月十五日，上午一開始為東京大學 Masatoshi Imada 的演講 Quantum Monte Carlo for strongly correlated systems，Quantum Monte Carlo 以我們外漢的背景知識頂多在成大第一原理會議聽過鄭靜教授的演講，此演講收穫頂多知道可以應用在 quantum liquids 跟 unconventional superconductivity，另外上午兩個大會演講為核物理的計算與預測颱風的行為，我的能力大概只聽的懂近代物理與普物的部分，總之只能很驚嘆不同領域的計算發展的應用，此外一提，午餐很不錯有日本的哈密瓜與巨峰葡萄，超好吃。下午的會議包含的很廣泛，有 K-computer、Quantum Monte Carlo、教育與計算物理、氣象疾病預測等等，大多以我的研究領域不同，而去找計算物理在教育的 section 聽演講，第一個講量測 entropy 很有意思，但以要教學上可能對於高中學生來說太難，第二位美國人他給了一個想法，美國教授從 1980s 開始教計算物理到現在隨著 google 發達學生的背景知識越來越多與不同類型，他就分享對於計算物理在現今的發展的思想，應該怎麼改變教育的方法與題材，有朝一日如果可以當老師的話是不錯的一個演講，第三個挪威演講者使用物理在數學、物理、統計等等上的課程教學，最後一個韓國人講基本粒子的計算應用，KEK 實驗與分析上面的結合，完全是隔行如隔山，不過有好友是做高能物理的聽一聽可以跟他們請教討論。

第二天十月十六日會議，早上會議有 Stefan Blügel 的演講，偶爾可以在第一原理領域 PRL 文章看到大師的研究，演講討論到 KKRnano、juRS、OpenMP 等等，這些計算都超越我能力所及的，不過沒關係可以多知道新研究的趨勢也是會議的意義之一，下午則是關於太陽能電池的計算演講。此外 CCP 會議的 guided tours 是參觀位於神戶人造島上的京電腦(K computer)當然非常的先進高科技，為 Fujitech 富士通公司所製造，捷運站還以 K computer 命名為「京コンピュータ前駅」，「京」的意思取中文 10 的 16 次方而非京都詩情畫意之類的，京電腦可以解決的人類問題也如同前面提到的氣象預測、奈米科技、生物基因工程等等，京電腦也是現在世界第二快的電腦，後來有興趣研究了一下 wiki 的資訊，得知台灣中央氣象局夠買了京電腦，成為首位用戶來增強台灣國內天氣預測的計算能力，跟其他研究員討論到製造京電腦的成本是現在世界最快的五倍，只能說美國人賣技術給海外然後自己擁有技術，用相對低成本製造更好的電腦，這可能是台灣學界與產業可以成長學習開發新事業的地方，也看到會議介紹京電腦的海報、實體電腦模組散熱管線還有很酷的八吋晶圓展示，對於日本的電腦科學進步真是給我上了一堂課。此次神戶會議，看到國際上在計算物理的各方面研究發展，跟神戶與日本關西的進步，不愧是先進國家在台北也體驗不到的都市潛文化，像是日本人的禮節或是對於工程、人造島、填海的關西機場與機場鐵路等等建設的遠見都是台灣所不及的。

會議第三天十月十七日，今天神戶早上開始下毛毛雨，回想起來那天會議結束回飯店雨下超大，氣溫大約二十度不到沒有雨傘情狀之下，意外的體驗神戶落湯雞之行。回到會議過程，早上演講為 K-computer 計畫背景與發展，之後是計算機、半導體與奈米科學發展的演講。今天下午選了 Quantum

Monte Carlo 的 section，值得一提是第二個演講者說的題目 Quantum Monte Carlo Simulation of Deconfined Critical Point，關於二維量子的自旋模型，考慮 spin1/2 的 Heisenberg model 跟多體的交互作用，i.e. J-Q model，到後來的 U(1)、SU(N)與 lattice critical symmetry 我就不太了解在 VASP 計算上可否運用上來，在物理上概念上可以了解臨界相變的問題，至於要應用到計算上就要向 QMC 的研究團隊拜師學藝了;另外今天要參加 poster section 我的號碼是 117 號海報，旁邊剛好也是新竹來的台灣團隊，旁邊則是印度團隊，剛到海報會場就有一個美國橡樹嶺國家實驗室的研究員跟董人銓博士討論海報論文，他與我們蠻多問題，也提供了我們一個免費的計算軟體 the Elk FP-LAPW Code，他說這可以推廣做到複雜系統的 spin wave，也可以在自己電腦安裝跑計算，之後有空的話可以採用他的建議嘗試看看用這軟體做計算，另外一個老外問的問題也是一樣他們似乎會問說 spin spiral 是 unit Cell 要重複變成 supercell 嘛？這可能也是海報沒有寫出 Sandranskii 的理論架構，容易誤解使人會錯意，這也是需要多學習的地方，如何利用有限空間的海報讓參加會議的研究員們了解所想要表達的，做海報也是一種藝術跟智慧。

會議最後一天十月十八日，前兩個講的是 DNA 跟天文，我是門外漢也只能當做科普 seminar 來聽，第三個演講者是朝日新聞的資深主編，由於女主編語言關係所以有同步翻譯人員與耳機，演講簡介 K-computer 在各個領域上的應用也得知台灣中央氣象局是首位 K-computer 的用會之類的，後來是 open discussion，各國教授研究員都討論蠻熱烈的，關於電腦科學在預測未來地震颱風，還有投資這麼多金費在電腦預知的效應上頭等等，我也只能從旁聽取大家意見，以我新手的觀點覺得似乎人類未來的議題還是很多，畢竟要更進步要付出的代價更高。最後一天午餐，又出現了哈密瓜，好吃！最後一天下午演講有另一個 DFT section，有三個跟 graphene 有關的，其中兩個 Hiroshi Mizuta JAIST 團隊的學生，會議的樂趣猜他們是來自哪個國家，以腔調來猜的話是馬來西亞或印尼人吧，長得也不像中國人，但他們演講完沒去證實我的預測是否正確，在研究上面他們團隊採用都是 non-equilibrium Green’ s function (NEGF) method 在 OpenMX 上計算 graphene 或 graphene nanoribben 的量子傳輸現象，當然也有在 graphene 有 defect 的系統之下做能帶計算，我想這些 defect 性質改變電子傳輸可以做來實驗上證實他們的預測。另外一個能帶計算的韓國人，討論以下材料 Sr_2IrO_4, Na_2IrO_3, and Li_2IrO_3 的磁性 SOC 與 LDA+U 的研究，他們預測有趣的地方在 Na_2IrO_3 有一般絕緣體會轉換成拓樸絕緣體的量子相變。


Fig. Nichii Gakkan conference center


Fig. 演講會場的雙投影幕

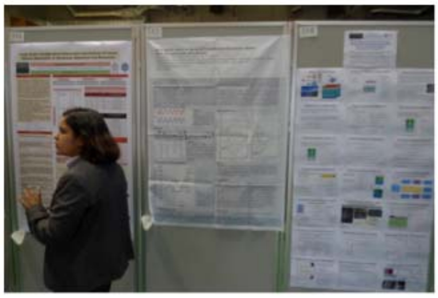


Fig. 會議海報張貼(中)

二、與會心得

這次計算機物理年會(CCP 2021)是我第一次出國開會，當然也很緊張於搭飛機還有日本複雜的電車所造成的迷路，還好事先請教了一些在大阪大學、東京附近留學的同學指導，可以順利抵達會場，也看到神戶的京電腦與聚集計算物理的科學家們或其他不同領域的計算科學家們，也品嚐到遠近馳名的神戶牛排，真是大開眼界，日本本質上還是個大國，這很容易看到一下飛機的基礎建設、科學研究、神戶港的建設，CCP計算會議上聽到很多不同領域的會議，earth science、atomic nucleus、laser fusion etc.

這些似乎都是物理應用上可以幫助人類更文明的領域，解決預測氣象、核融合解決能源問題等等，看似基本的問題卻得到日本科學界的重要關注，像是最近的颶風珊迪重創部分美東，在在顯示這些物理在地球科學等等議題的重要性(如第一天上午會議演講Challenge toward the precipitation of typhoon behaviour and down pour)，因此藉由這次機會在神戶看到國際上科學科技所關注的問題，真是不虛此行這自己的眼界更加多元與前瞻性。

雖然parallel sessions演講的題目廣泛，像是第二天與最後一天都有DFT的演講section，第二天一部分演講爲電池的計算應用，最後一天主要是graphene的計算研究，可以看到不同於自己團隊的研究就是參加會議值回票價的地方，也第一次在國外的國際會議跟外國人討論自己的研究或是他們的研究，這次在會議認識的橡樹嶺實驗室研究員，也感謝他對於我的研究提出改善的地方與未來可以做的研究方法，也在自己研究上面可以增加經驗的地方，還有在大阪梅田車站問路時遇到一個英文超級好的日本留加拿大女生大力協助，似乎也是這次會議行程有趣的意外插曲！

三、發表論文全文或摘要

Abstract. Nanostructured magnetic materials have recently received enormous attention because of their fascinating physical properties and potential applications. For example, finite free-standing gold atomic chains were first reported in 1998 [1,2], and their physical properties, such as the actual length of the chains have been the focus of intensive experiments and theoretical studies since then. Physically stable magnetic nanowires deposited on metallic substrates are one of the most important nanostructures and a variety of techniques have been used to prepare and study them. In particular, Gambardella et al [3,4] succeeded in preparing a high density of parallel atomic chains along steps by growing Co on a high-purity Pt (997) vicinal surface. The magnetism of the Co wires was also investigated by the x-ray magnetic circular dichroism. [4].

We have recently performed *ab initio* studies of the physical properties of linear 3d transition metal atomic chains [5, 6], and found that Fe and Ni linear chains have a gigantic magnetic anisotropy energy [5] and that stable spin-spiral structures are formed in the V, Mn and Fe linear chains [6]. In order to investigate how the structural distortion may affect the spin-spiral waves of the nanowires, here we report our *ab initio* calculation of the total energy of transverse spin-spiral waves as a function of the wave vector as well as other magnetic properties for the zigzag 3d transition metal atomic chains. Firstly, we find that there are both the acoustic and optical magnons in the atomic zigzag chains. Secondly, we find that the Cr, Mn and Fe zigzag chains have a stable spin-spiral wave at equilibrium structure, while the magnetic ground state of the Sc, Co and Ni chains remains collinear. The spin-wave stiffness constant and also the magnetic phase transition temperatures of these 3d metal zigzag chains are also evaluated.

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[3] P. Gambardella, et al., Surf. Sci. 449, 93 (2000).

[4] P. Gambardella, et al., Natureu 416, 301 (2002).
[5] J. C. Tung and G. Y. Guo, Phys. Rev. B 76, 094413 (2007).
[6] J. C. Tung and G. Y. Guo, Phys. Rev. B 83, 144403 (2011).

四、建議

五、攜回資料名稱及內容

會議手冊、會議論文集隨身碟(elecom，made in Taiwan)、神戶相關導覽

六、其他

感謝國科會提供經費補助出國以及郭光宇教授、董人詮學長的大力幫忙

國科會補助計畫衍生研發成果推廣資料表

日期:2013/01/09

國科會補助計畫	計畫名稱: 電漿子奈米材料之電磁理論與模擬研究
	計畫主持人: 郭光宇
	計畫編號: 100-2112-M-004-002- 學門領域: 光電物理－理論

無研發成果推廣資料

100 年度專題研究計畫研究成果彙整表

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	技術移轉	件數	0	0	100%	件	
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	參與計畫人力（外國籍）	碩士生	0	0	100%	人次	
		博士生	0	0	100%		
		博士後研究員	0	0	100%		
		專任助理	0	0	100%		
其他成果 (無法以量化表達之成果如辦理學術活動、獲得獎項、重要國際合作、研究成果國際影響力及其他協助產業技術發展之具體效益事項等，請以文字敘述填列。)		無					

	成果項目	量化	名稱或內容性質簡述
科教處計畫加填項目	測驗工具(含質性與量性)	0	
	課程/模組	0	
	電腦及網路系統或工具	0	
	教材	0	
	舉辦之活動/競賽	0	
	研討會/工作坊	0	
	電子報、網站	0	
	計畫成果推廣之參與（閱聽）人數	0	

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）

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）