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國立交通大學
National Chiao Tung University

出國報告（出國類別： 國際會議及學術交流）

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參加第 23 屆拉曼光譜學國際會議暨出訪印度科學理工學院、貝拿勒斯印度教大學

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前往國家：印度科學理工學院、貝拿勒斯印度教大學
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一、摘要（200-300 字）

The purpose of the visit to India is to attend the 23rd International Conference on Raman Spectroscopy (ICORS) and to visit Prof. Umapahy at Indian Institute of Science, Bangalore, and Prof. Saha at Banaras Hindu University, Varanasi, in the scope of gaining new insights into our research topics as well as of seeking new research collaborations that may expand our research in new directions. To achieve the above-mentioned purpose, I attended the ICORS meeting (Aug. 12 - 17) and gave an oral presentation of our recent research progress. I had many intensive and stimulative discussions on topics both general and related to our research with many attendees who are experts in the field of Raman spectroscopy. After the conference, I visited Laboratories of Prof. Umapahty (Aug. 18 - 20) and Prof. Saha (Aug. 21 – 23.) I inspected the ultrafast time-resolved spectroscopic system developed there, and had discussions with many researchers including, Professors, post doctoral fellows and students. I discussed possible research collaboration with Prof. Saha and decided to start working on a new project in which we investigate new materials that Prof. Saha provides with our spectroscopic systems developed at NCTU.

這次出訪印度的目的是參加第 23 屆拉曼光譜學國際會議(ICORS 2012)並拜訪位於邦加羅爾的印度科學理工學院的 Umpahy 教授以及位於瓦拉納西的貝拿勒斯印度教大學（Banaras Hindu University）的 Saha 教授，以使我們的研究主題獲得新的見解以及尋找可能會為我們的研究計畫擴展新方向的新的共同研究。為了達到那些目的，我參加 ICORS 會議(8 月 12 日-17 日)並在會上針對最近的研究成果進行口頭發表。我和許多出席會議的拉曼光譜學領域專家深入討論了一般的以及和我們研究計畫相關的主題。在會議結束後，我拜訪了 Umapahty 教授(8 月 18-20 日)及 Saha 教授(8 月 21-23 日)的實驗室。我在那檢視那裡的超快時間解析光譜系統，並和眾多研究學者進行討論，像是那裡的教授、博士後研究員及學生們。我和 Saha 教授討論將來可能進行的共同研究，並決定開始藉由 Saha 教授提供可以在交通大學的光譜系統使用的新的材料實行一項新研究。

二、目次

三、本文

（一）目的

The first purpose of the visit to India is to attend the 23rd International Conference on Raman Spectroscopy (ICORS) to have discussions on our recent research achievements with the world finest experts of Raman spectroscopy and to gather information of the recent advancements and trends in the field. The main aim of those activities is to gain new insights into our research topics so that we can further promote our studies into the direction that has higher impact on the field. The second purpose is to visit Prof. Umapathy and Dr. Venkatesh at Indian Institute of Science, Bangalore and Prof. Saha at Banarasu Hindu University, Varanasi. The main aims of those visits are to study one of the world most advanced research instrument, femto-second time-resolved Raman loss spectroscopic system, and to seek future collaborations that may expand our research in new directions.

此次出訪的第一個目的是參加第 23 屆拉曼光譜學國際會議(ICORS 2012)，在那裡和拉曼光譜學的世界頂尖專家們討論我們最新的研究成果，並收集此領域最新進展及趨勢的相關資訊。參與這些活動最主要目標是為我們的研究主題增加一些新的見解，讓我們的研究提昇到領域中有較高影響力的方向。第二個目的是去拜訪位在邦加羅爾的印度理工學院的 Umapathy 教授和 Venkatesh 博士，以及位於瓦拉納西的 Banarasu Hindu University 的 Saha 教授。兩次出訪的主要目標是針對世界上最先進的研究儀器之一，飛秒時間解析拉曼損失光譜系統進行研究學習，並尋找未來可能為研究擴展新方向的共同研究。

（二）過程

The following is the schedule of my trip:

Aug. 12	14:25	Depart from Taipei (桃園) (SQ877) 飛離台灣
	20:00	Transition at Singapore (SQ502) 新加坡轉機
	22:00	Arrive in Bangalore 抵達邦加羅爾
Aug. 13	8:00 – 19:00	ICORS 1st day
Aug. 14	8:00 – 19:00	ICORS 2nd day
	12:45 – 13:05	Give oral presentation, “Solute-solvent multipole interactions as the origin of intermolecular vibronic intensity borrowing in resonance hyper-Raman scattering,” in Novel Raman instrumentation and techniques session. 於「新穎拉曼設備及技術」議程中進行題為”Solute-solvent multipole interactions as the origin of intermolecular vibronic intensity borrowing in resonance hyper-Raman scattering”的口頭發表
Aug. 15		ICORS 3rd day (Indian national holiday; no academic events) ICORS 第三天(印度國定假日)
	11:00 – 12:00	Preparation of ppt slides for the seminar in Varanasi. 準備將於瓦拉納西的會議上使用的投影片
Aug. 16	8:00 – 15:00	ICORS 4th day 會議進行第 4 天
Aug. 17	8:00 – 18:00	ICORS 5th day 會議進行第 5 天
Aug. 18	11:00 – 13:00	Visit IISc and discussion with Dr. Venkatesh at Indian Institute of Science. 拜訪印度科學理工學院並和 Dr. Venkatesh 進行討論
Aug. 19	17:00 – 18:00	Inspection of ns-time resolved system and discussion with Prof. Umapathy’s student 觀測 ns-時間解析系統並和 Umapathy 教授的學生們進行討論

Aug. 20	13:00 – 17:00	Visit IISc and inspection of their ultrafast laser facilities. Discussion with Dr. Venkatesh and Dr. Roy 拜訪 IISc 並觀察他們的超快雷射設施。和 Venkatesh 博士及 Roy 博士進行討論
Aug. 21	8:45	Depart from Bangalore (SG-224) 飛離邦加羅爾
	13:40	Transition at Delhi (SG-114) 於德里轉機
	15:00	Arrive in Varanasi 抵達瓦拉納西
Aug. 22	11:00 – 12:00	Inspection of Prof. Saha's laboratory 參觀 Saha 教授的實驗室
	13:00 – 15:00	Discussion with Prof. Saha's student 和 Saha 教授的學生進行討論
	15:00 – 17:00	Discussion with Prof. Saha 和 Saha 教授進行討論
Aug. 23	11:00 – 13:30	Discussion with Prof. Saha 和 Saha 教授進行討論
	16:00 – 18:00	Department seminar "Raman and Hyper-Raman Spectroscopy: Basics and Applications"
Aug. 24	12:40	Depart from Varanasi (SG-221) 飛離瓦拉納西
	23:30	Transition at Delhi (TG-316) 於德里轉機
Aug. 25	7:10	Transition at Bangkok (TG-634)
	11:50	Arrive in Taipei (Taoyuan) 抵達台灣

8 月 12 日，星期日：搭機前往印度邦加羅爾。

Aug. 13th, Mon: I mainly attended "Raman application to biological cells and tissues" and "Femtosecond Stimulated Raman Spectroscopy" sessions.

The lecture "Femtosecond Stimulated Raman spectroscopy" given by R. A. Mathis nicely reviewed recent developments of femto-second stimulated Raman Spectroscopy (FSRS) technique, which is now expanding its field from proof of the principle experiments to a valuable tool in studying dynamic behavior of molecules in ultrafast time regime. He showed the capability of FSRS with several examples, such as excited state proton transfer in the green fluorescent protein (GFP), excited state

charge transfer reactions that form contact ion pairs in non-covalent donor-acceptor pi-complexes, and the mixed inversion-rotation isomerization mechanism of the isomerization of an azobenzene analog.

Several other lectures in the “Femtosecond Stimulated Raman Spectroscopy” provided us some new experimental techniques that may be useful in our research project with hyper-Raman spectroscopy. Those include, high throughput conversion of the excitation femto-second laser pulse into pico-second pulse by “spectral compression” with long second-harmonic generation (SHG) crystal. It is noteworthy that the technique is capable in the ultraviolet wavelength region.

8 月 13 日,星期一：我主要時間都待在標題為「拉曼於生物組織及細胞之應用」(Raman application to biological cells and tissues) 及「飛秒激發拉曼光譜學」(Femtosecond Stimulated Raman Spectroscopy)的議程裡。

由 R.A. Mathis 帶來的演講“(飛秒激發拉曼光譜學)Femtosecond Stimulated Raman Spectroscopy”回顧了飛秒激發拉曼光譜學(FSRS)技術近期的發展，這項技術現在將其領域從原理實驗的考證擴展到身為研究分子在超快時間製法中的動力行為(dynamic behavior of molefules in ultrafast time regime)的珍貴工具。他以幾個例子展示 FSRS 的性能，像是綠螢光蛋白(green fluorescent protein, GEP)的激發狀態質子轉移、無共價鍵 donor-acceptor pi-complex 組織親密離子對的激發狀態電荷轉移反應，以及類偶氮苯的異構化反應的混合反轉旋光性(inversion-rotation)異構化過程。

“飛秒激發拉曼光譜學”議程中的其他演講提供了一些或許可以在我們的超拉曼光譜學研究計畫中使用的新實驗技術。包含.由「spectral compression」和二次諧波(second-harmonic generation , SHG)水晶的激發飛秒雷射脈衝進入微微秒(pico-second)脈衝的高通量轉換。很值得一提的是這項技術可以使用在紫外線波長的領域。

Aug. 14th, Tue: I gave an oral presentation, “Solute-solvent multipole interactions as the origin of intermolecular vibronic intensity borrowing in resonance hyper-Raman scattering,” in Novel Raman instrumentation and techniques session. (Fig. 1) After the presentation, I had discussion on my research subject with many researchers including, Prof. Bin Ren of Xiamen Unicversity, Prof. Mizutani of Osaka University, Prof.

Umapahty of Indian Institute of Science and Prof. Furukawa of Waseda University. The discussed matters include possibility of generalizing the observed intermolecular intensity borrowing through multipole interaction to other spectroscopies such as conventional linear Raman scattering, common nature of the molecular species that exhibit intermolecular intensity borrowing phenomenon, possible modification to the experimental setup for higher signal detection sensitivity, and possibiliy of involvement of molecular polarizability.

8 月 14 日，星期二：我在這天進行了口頭發表，題目是「Solute-solvent multipole interactions as the origin of intermolecular vibronic intensity borrowing in resonance hyper-Raman scattering」，位於「新穎拉曼設備及技術」(Novel Raman instrumentation and techniques)議程裡。(請見圖一) 發表結束後，我和許多研究學者討論我的研究報告，包括 Xiamen 大學的 Bin Ren 教授、大阪大學的 Mizutani 教授、印度科學理工學院的 Umapahty 教授以及早稻田大學的 Furukawa 教授。討論的議題包含歸納出像是傳統線性拉曼散射的其他光譜學觀測到的分子間的強度多重互動的可能性、普遍分子種發展出分子間的強度的各種現象等等。

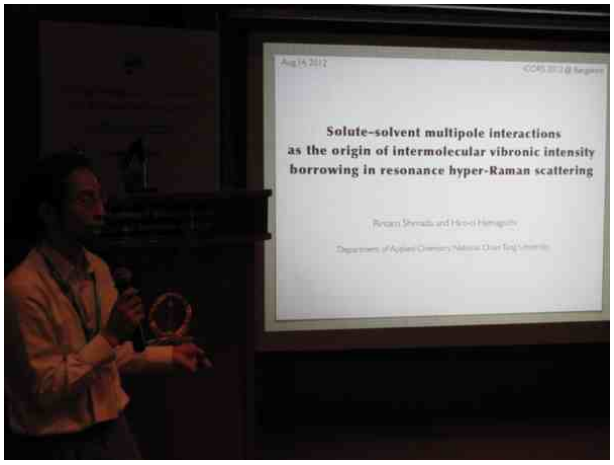

Fig. 1. Presentation at ICORS-2012
圖一. 我於 ICORS 2012 的發表

Aug. 15th, Wed: Since there were no academic events scheduled for the day, I spend some time to review the abstracts of presentations on 4th and 5th days of ICORS. I also made preparation of ppt slides for the seminar in Varanasi.

8 月 15 日,星期三(印度國定假日)：由於大會這天沒有安排任何的學術活動，我便花了點時間閱覽會議第四天及第五天的發表論文摘要。同時也為我之後在瓦拉

納西的研討會上要使用的 ppt 投影片做準備。

Aug. 16th, Thu: I mainly attended “Biomedical application of Raman spectroscopy” and “Ultrafast Raman spectroscopy – II” sessions.

It seems that the current trend of Raman application in the biomedical field is shifting from imaging of cellular/tissue samples towards mass processing of hundreds of spectra to extract characteristic spectroscopic signature of marker molecules/ biological events. The analytical methods they utilize are many different variations of multivariate analysis, however, the extracted spectral information are often hard to interpret. I found lecture “SERS of biological cells: A novel probe of metabolomics and hemoglobin” presented by L. D. Ziegler quite interesting. In the lecture, he discussed the multivariate analysis of Raman spectra of vegetative bacterial cells obtained with surface enhanced Raman spectroscopic (SERS) technique. The largest components of the signals are found to result from molecules involved in the purine degradation or salvation pathway which are concentrated at the outer layers of these cells. He showed good correspondence of the SERS spectra of the major component from cell with those of adenine, hypoxanthine, guanine, and other metabolites. The work showed the SERS capability of detecting and investigating extracellular metabolome. At the same time, the work illustrated the limitation of the SERS technique to *in vivo* study that it can only detect few molecular species at the very outer surface of the cell.

8 月 16 日，星期四：我出席了「拉曼光譜學於生物醫學上的應用」(Biomedical application of Raman spectroscopy)及「超快拉曼光譜學-II」(Ultrafast Raman spectroscopy)議程。

目前拉曼在生物醫學領域應用的趨勢似乎從細胞/組織的樣本成樣移轉到大量處理幾百種光譜以取得標的分子/生物結果特有的光譜特徵。他們所使用的分析方式比起多變數分析有相當多的變動，然而，取得的光譜資訊通常都很難去做解釋。我對於 L. D. Ziegler 的演講「SERS of biological cells: A novel probe of metabolomics and hemoglobin」相當感興趣。在該演講中，他探討使用表面增強拉曼散射(SERS)技巧得到的植物細菌細胞拉曼光譜的多變數分析。研究發現其中所構成的最大訊號是從嘌呤的代謝或者是從這些細胞外層濃縮而來的 salvation pathway 中找到的。他展示如腺嘌呤、次黃嘌呤、鳥糞嘌呤及其他代謝物的主要細胞構成的 SERS 光譜，以及 SERS 於偵測及研究細胞外的代謝物組的能力。同

時，他的研究也描繪出了 SERS 技術於活有機體研究上的限制，在細胞的極外側它只能夠偵測出少數分子種。

Aug. 17th, Fri: Mainly attended “Clinical application of Raman spectroscopy” and “Ultrafast Raman spectroscopy–III” session.

The lecture by P. Kukura “Time-domain vibrational spectroscopy of excited electronic states” showed series of novel approach towards impulsive stimulated Raman spectroscopy and presented the broadband and highly resolved time-domain Raman spectra of excited electronic states. Their new technique is based on iterative processing of both time-domain and spectral-domain information to almost completely eliminate the background signals arisen from solvents as well as the target molecules in the ground state.

8 月 17 日，星期五：參加「拉曼光譜學的應用」(Clinical application of Raman spectroscopy)及「超快速拉曼光譜學-III」(Ultrafast Raman spectroscopy-III)議程。

P. Kukura 的演講「Time-domain vibrational spectroscopy of excited electronic states」展示了一系列脈衝激發拉曼光譜學的新穎方法，並提出電子激發態的寬帶及高時間區域解析拉曼光譜。他們的新技術是根據時間及光譜區域的反覆式流程資訊，幾乎能完全排除溶劑及基態目標分子所產生的背景訊號。

Aug. 18th, Sat: I visited Dr. K. Venkatesh at Indian Institute of Science, Bangalore to discuss the recent progress of there Raman application to clinical and biomedical diagnosis.

8 月 18 日,星期六：我拜訪了邦加羅爾的印度科學理工學院的 Venkatesh 博士，和他討論臨床及生物醫學診斷上拉曼應用近來的進展。

Aug. 19th, Sun: I visited Prof. Umapathy’s laboratory. There I inspected nano-second time-resolved Raman spectroscopic system and discussed with the Prof. Umapathy’s students. There apparatus are, though it is based on rather old technologies, well organized.

8 月 19 日，星期日：我拜訪了 Umapathy 教授的實驗室。在那裡我檢視了十億分之一秒時間解析拉曼光譜系統，並和 Umapathy 教授的學生們進行討論。他們的儀器設備雖然是使用較舊的技術製成的，但是組織良好。

Aug. 20th, Mon: I inspected femto-second time-resolved Raman loss spectroscopic system developed there. The system is one of the most advanced femto-second Raman loss system, with one laser amplification and two independent optical parametric amplification system to manipulate the wavelength of three laser beams independently. The femto-second to pico-second conversion of the Raman pump pulse is realized by 4f-dispersive geometry with mechanical slit, of which conversion efficiency are a few percent. The system is well designed and neatly organized so that most of the optics are easily accessible for the fine alignment. (Fig 2.)

After inspecting the system, I discussed with Dr. K, Venkatesh and Dr. K. Roy on their recent results obtained with the instrument. We also discussed the possibility of incorporating computational approach, such as quantum chemical computation and/or molecular dynamics simulation, into our experimental approach on the investigation of intermolecular interaction in liquids.

8 月 20 日，星期一：這天我檢視了這裡的飛秒時間解析拉曼光譜系統。這個系統是最先進的飛秒拉曼系統之一，有一個雷射放大和兩個獨立的光學參量放大系統去操作三道獨立的雷射光束波長。使用 4F-分散的幾何形狀與力學切縫可以瞭解拉曼幫浦脈衝由飛秒轉變至微微秒的過程，此種轉變比一般來得有效率幾個百分比。這個系統設計相當良好有組織，所以光學元件可以輕易的進入進行校準。(請見圖 2)

在觀測完該系統後，我和 K.Venkatesh 博士和 K.Roy 博士進行關於他們最近得到的數據結果進行討論。我們還討論了將像是量子化學計算，或是分子動態模擬合併使用我們的液體分子間互動實驗方法的可能性。

Fig. 2. Femto-second system with Dr. Venkatesh.
圖二 Venkatesh 博士和飛秒系統

8 月 21 日，星期二：搭機離開邦加羅爾，於德里轉機，抵達瓦拉納西。

Aug. 22nd, Wed: I visited Prof. Saha at Banaras Hindu University. There I inspected their research facilities for chemical synthesis and analysis. The spectroscopic apparatus at their department are limited to only the basic instruments such as UV/VIS absorption, infrared absorption and fluorescence spectrometers. Prof. Saha's laboratory has expertise in the synthesis of various types of new compounds such as ionic liquids, polymer films, catalytic molecular complexes, etc. Although they are very much interested in investigating into the novel properties of their newly synthesized materials, it was not possible due to the lack of advanced spectroscopic instrumetns. We discussed on the possible research collaboration and decided to start working on a new project in which we investigate on new materials that Prof. Saha and their group members synthesized by our spectroscopic systems developed at NCTU. (Fig. 3)

8 月 22 日，星期三：我拜訪了 Banaras Hindu University 的 Saha 教授。在那裡我觀摩了他們綜合及分析化學使用的研究設施。他們系上的光譜儀器只能夠做像是 UV/VIS 吸收作用、紅外線吸收作用及螢光光譜儀等的基本測量。Saha 教授的實驗室擅長綜合多種類型的新化合物像是離子液體、聚合物膜、催化劑分子複合物等等。雖然他們對於使用新穎的道具研究新的綜合原料，但是卻因缺乏進階的光譜儀器而無法達成。我們討論未來可能進行的共同研究，並決定開始進行一項新的計畫：使用我們於交通大學的光譜系統設備來研究 Saha 教授團隊所整理出來的新材料。(請見圖 3)

Fig. 3. With Prof. Saha and his students.
圖三. 與 Saha 教授和他的學生們合影

Aug. 23rd, Thu: I was given an opportunity to present a lecture to the faculty members and students in the Department of Chemistry, Banarasu Hindu University. I gave a 60 minute talk titled as “Raman and Hyper-Raman Spectroscopy: Basics and Applications,” in which both experimental and theoretical basics of Raman and hyper-Raman spectroscopy was reviewed with many of our own research results used as examples. The audience was quite active during the talk and I received many responses from both Professors and students. Few of the discussions we had afterward the lecture include, application of the hyper-Raman and Raman spectroscopy into biological science, physical interpretation of intermolecular interaction that facilitates intermolecular vibronic coupling, possibility of utilizing time-resolved measurement of the intensity borrowing phenomenon to get deeper insight of the coupling mechanism, and mixed solvent measurement to further extract information on solute–solvent interactions. (Fig. 4)

8 月 23 日，星期四：我有幸得到在 Banarasu Hindu University 化學系對他們的師生進行演講的機會。我進行了題為「Raman and Hyper-Raman Spectroscopy: Basics and Applications」的 60 分鐘左右的演講，其中包含了拉曼及超拉曼光譜學的實驗及理論資料，且由我們的研究計畫中取了很多例證。聽眾們在演講過程中反應相當踴躍，我從教授及學生們那得到許多回應。我們在演講後進行的討論包含超拉曼及拉曼光譜學在生物科學上的應用、促使分子間電子振動聯繫的分子間互動物理詮釋、利用時間解析測量強度以更加深入瞭解連結機制等。(請見圖 4)

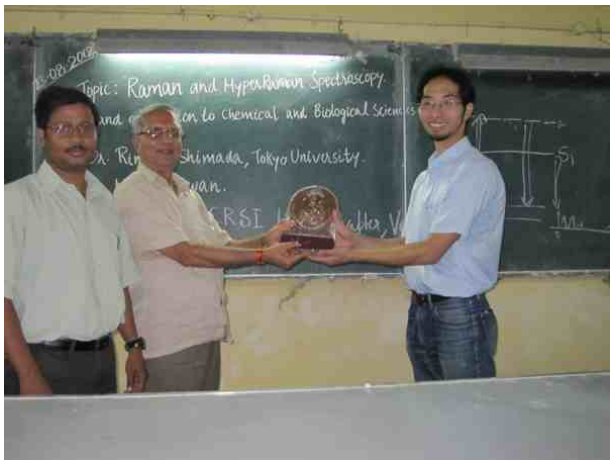

Fig. 4. At the lecture, with Prof. Saha and Prof. Singh.
圖四. 演講後和 Saha 教授和 Singh 教授合影

8 月 24 日、25 日，星期五、六：搭機返回台灣。

（三）心得及建議

The visit to ICORS conference and the visit to both Indian Institute of Science and Banaras Hindu University were very much stimulating, insightful and meaningful to our research project. I was able to gather much information that were new and were not available to us before. Those new information broadened my point of view on our own research topic and help me gain a new insight into our topic. In addition, through the discussion with many researchers from around the world and by listening to many advanced lectures, I strongly felt that the scientific area that Raman spectroscopy can contribute is now rapidly expanding. The development of new methodologies specially designed to each of those varieties of scientific problems will be a key factor for taking lead of those expansions to new fields.

這次參加 ICORS 會議及出訪印度科學理工學院和 Banaras Hindu University 讓我感到受益良多。收集到了許多嶄新的資訊。那些新資訊擴展了我的視野，並讓我對目前進行的研究有了一些新的看法。此外，透過和許多來自世界各地的研究學者進行討論並參與許多進階演講，我強烈地感受到拉曼光譜學可於科學界貢獻的部份正在迅速的擴展當中。