國立交通大學
National Chiao Tung University

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出國報告（出國類別：☐ A類、考察訪問
■ B類、出國短期研究
☐ C類、國際會議

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Research visit: "Collaborative research work on the physical and chemical properties of carbon nanostructures"

研究訪問："物理和化學性質碳納米結構的合作研究"

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前往國家：日本/名古屋/名古屋大學
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備註：出國報告書審核程序如下
一、初閱：各學院教師A、B、C類及其他行政單位A類由單位主管，研究生由指導教授；中心計畫及學群A、B、C類由各中心計畫主持人。
二、複閱：經費所屬之一級單位；中心計畫及學群A、B、C類由頂尖計畫執行長。

一、摘要 Summary

A collaborative visit to the research laboratory of Professor Stephan Irle at Nagoya University was mainly focused on pursuing the existing research projects and planning new collaborations. The time in Nagoya was spent in a very energetic way, writing up resulting manuscripts, deciding the content of new manuscripts, and discussing with Prof. Irle and his students the direction of future efforts.

此次訪問日本名古屋大學 Stephan Irle 教授主要希望能延續現有的研究計畫並研討新的合作內容，行程內容主要是撰寫研究成果並與 Irle 教授及其學生討論未來研發的方向。

二、本文

（一）目的及過程

In the period February 7–17, 2011, I was invited for 10 days visit in the laboratory of professor Stephan Irle at the Institute of Advanced Research and the Department of Chemistry of Nagoya University in Nagoya, Japan. The primary reason of the visit was the shared collaborative effort oriented toward finalization of currently lasting research project and planning and coordination of new projects being the continuation of our work on the physical and chemical properties of various nanostructures, mainly composed of carbon atoms. The present visit to Japan was also very important to clarify a number of disputable question originated from the student exchange between our two groups: Yoshifumi Nishimura visits to Hsinchu and Wunfan Li visit to Nagoya. Another important aspect of the visit was writing the publication describing the application of the SCC-DFTB method to various aspects of physics of carbon nanotubes and fullerenes. During the stay in Japan, I was lodged in the Symposion lodging facility, conveniently located on the campus area within a walking distance from the Institute of Advanced Research of Nagoya University. A laboratory spare key and an electronic access card enabled working at the Institute even outside of regular working hours.

在 2011 年 2 月 7~17 日這十天的時間當中，我訪問了 Stephan Irle 教授位在日本名古屋大學 Institute of Advanced Research and the Department of Chemistry 的實驗室，最主要的訪問動機是為了分享我們彼此在碳主體的多樣奈米結構物性和化性研究上的最新成果和討論新的合作計畫。這次日本訪問另外一個相當重要目的是討論我們兩個團隊之間交換學生的問題(該團隊的學生 Yoshifumi Nishimura 來台和我們實驗室的李文凡同學赴日學習)；其他還有撰寫發表有關於電荷自洽密度泛函緊束縛法(SCC-DFTB)在多種碳奈米結構和富勒烯物理方面的應用。在日本的這段期間我住在距離校園附近的 Symposion 宿舍，並擁有實驗室的鑰匙和電子感應卡，使我在正常上班以外的時間也能到實驗室工作。

（二）心得及建議 What has learned/suggestion

The collaboration between professor Irle and me dates back to 2003, when we both spent few years in the group of professor Keiji Morokuma at the Emory University in Atlanta, USA. At that time, professor Irle was a right hand of professor Morokuma, responsible for the projects related to nanostructures and I was a post-doctoral fellow in the same group. The collaboration concerned various aspects of chemistry and physics of carbon fullerenes and nanotubes, including their aggregates. Since that period, we have been working together on many interesting problems and coauthored a number of scientific papers. The collaboration is very dynamic and the already published papers result in new ideas leading to new publications. The present visit in Nagoya was mainly oriented toward finishing our two recent collaborative efforts. The first of them is devoted to explaining the unusual screening properties of carbon nanotubes and fullerenes, which almost completely extinguish the IR activity of molecules encapsulated inside them. This observation has profound importance for experimental characterization of encapsulated species (e.g., peapods). The resulting manuscript is currently undergoing the review process in the Journal of American Chemical Society and should be published soon. The second effort concerns the issue of explaining the experimentally observed abundance of fullerene and nanotube isomers. Our groups, together with collaborators from Krasnoyarsk, Russia, developed a kinetic stability model, which for the first time in the history of fullerene research was able to correctly predict the higher abundance of C_{60} in comparison to C_{70}; all previous efforts, based mainly on thermodynamic quantities, predicted the relative abundance in incorrect, opposite order. During the visit in Nagoya, we were working very intensively on a redaction of a manuscript suitable for Physical Review Letters, which is probably an appropriate place for publishing such a ground-breaking discovery. The manuscript is ready and will be submitted within a few days to PRL. Another topic we have been working during the visit concerns the physics of Goldberg fullerenes. The work on this project is already pretty advanced and we need just a few new data to start writing the resulting manuscript. During the visit we have discussed and planned how to obtain these new data, closely related to the topology and geometry of carbon networks in these very interesting molecular systems. In addition to the discussed here three scientific projects, we have spent considerable time on planning new scientific collaborations including expanding the kinetic stability model to large fullerene cages, modeling dynamical IR and Raman spectra obtained via Fourier transform of appropriate autocorrelation functions obtained from SCC-DFTB calculations,

and explaining the missing CO and benzene ring activity in the sum-of-frequency generation spectroscopy of polymeric PMMA and polystyrene deposited on single graphene sheets by performing appropriate molecular calculations with the SCC-DFTB method.

我和 Stephan Irle 教授的合作關係可追朔到 2003 年，當時在美國亞特蘭大的 Emory 大學裡，我們同時在 Keiji Morokuma 教授的團隊下工作了數年。當時 Irle 教授是 Morokuma 教授相當得力的助手，並從事奈米結構的研究，而我則是該團隊的博士後研究員，我們進行了關於碳富勒烯、奈米碳管在化學和物理方面的合作研究，從那時起，我們就時常一起工作，並一同發表了許多論文，當時的合作非常密切，發表的論文也激發了許多創新的想法。

這次訪問名古屋，我們主要完成了之前的兩個合作計畫，第一部分，他們致力於解釋奈米碳管和富勒烯不尋常的屏蔽效應，若將分子放在碳管內，其紅外線光譜訊號幾乎被遮蔽，這種效應對於封裝於奈米碳管分子的特性研究非常重要(例如探針)，這項研究結果已經投稿到美國化學會的期刊，很快將會被發表。第二部分則是解釋實驗上觀察到的多樣富勒烯和奈米碳管的結構，我們的團隊和俄羅斯的 Krasnoyarsk 教授發展了動力學穩定模型，它是在富勒烯的研究史上第一次能夠準確預測 C_{60} 和 C_{70} 的豐富度(在過去，若純粹由熱動力學特性去預測，往往會得到錯誤或相反的結果)。這次在名古屋的訪問過程中，我們非常謹慎的參考過去的文獻內容，認為這是適合發表的突破性發現，並準備在幾天後寄給 Physical Review Letters。在其他研究主題方面，我們還有針對戈德堡富勒烯(Goldberg fullerenes)進行研究，這項研究工作已經完成的差不多了，只需要一些新的數據就可以開始準備撰寫成果報告，由這次的訪問，我們討論並計畫如何取得這些新數據，像是利用這些有趣化學系統中的拓樸與碳分子網絡幾何結構。

三、附錄 Appendix