行政院國家科學委員會專題研究計畫 成果報告

子計畫一：飛秒超強光雷射化學之研究；子計畫二：有機太陽能電池光物理之研究

研究成果報告(精簡版)

計畫類別：個別型
計畫編號：NSC 98-2113-M-009-009-
執行期間：98年08月01日至99年10月31日
執行單位：國立交通大學應用化學系（所）

計畫主持人：林聖賢
共同主持人：寺西慶哲

處理方式：本計畫可公開查詢

中華民國 99年12月25日

〔中文摘要〕

關鍵字：量子控制，埃秒過程，強場游離—解離，高壓效應，全從始計算，內轉換，輻射性躍遷，圓錐交點

本計畫分為兩大部分。第一部分：我們持續進行高功率雷射相關研究，特別著重以飛秒雷射探究空氣中燈絲放射螢光、超激發態氧和其中性解離過程。我們也以理論方式研究線性偏極雷射脈衝照射下，對掌性分子中光致 π 電子旋轉與分子振動間的非絕熱耦合。此外我們也利用強場雷射，設計在飛秒時域中對於分子型離子進行電子定域化控制的方法。

第二部分：我們聚焦於原型分子 S_0－S_1 電子態間內轉換、吸收與螢光光譜的第一原理計算，已完成甲醛與苯兩種分子的研究。我們也研究了高壓效應（最高達 1.7 GPa）對於溶液中 LDS 698 分子超快能量馳豫的影響，即壓力調校。此外，我們開始研究化學反應中的非簡諧效應，迄今已完成非簡諧效應對於吡啶分子吸收與螢光光譜，以及對於分子團簇解離的影響。

〔Abstract〕

Keywords: quantum control, attosecond processes, intense-field ionization-dissociation, high-pressure effect, ab initio calculations, internal conversion, radiative transitions, conical intersection

The present project is divided into two parts:

In Part I, we continue our studies of high-power laser science. In particular, we investigate the fluorescence emitted from filament in air and super-excited states of oxygen and its neutral dissociation using femtosecond laser. We also theoretically studied the nonadiabatic couplings between optically induced π-electron rotations and molecular vibrations in a chiral molecule irradiated by a linearly polarized laser pulse. Furthermore, we have designed a method for controlling electronic localization in a molecular ion on an attosecond time scale using a high-intensity laser.

In Part II, we have focused our attention on the first-principle calculations of internal conversions, absorption spectra and fluorescence spectra between S_0─S_1 of prototype molecules. Two molecules, formaldehyde and benzene have been studied. We have also studied the effect of high pressure in a range of up to 1.7 GPa on ultrafast energy relaxation of LDS 698 in solution (that is, the pressure tuning). Furthermore, recently we have initiated the project of the anharmonic effect in chemistry. So far we have accomplished the anharmonic effect of the absoription and fluorescence spectra of pyridine molecule and the anharmonic effect on the dissociation of molecular clusters.

Part Ⅰ Investigations of Femtosecond High Power Laser Chemistry **飛秒超強光雷射化學之研究**

Ⅰ.1 Introduction

Recently we have initiated two quantum control projects. The first one is related to the control of the direction of the ring currents in benzene-like chiral molecule, which resulted in a PRL paper. The second one is for controlling electronic localization in a molecular ion on an attosecond time scale using high-intensity laser.

Ⅰ. 2 Results

We theoretically investigated the nonadiabatic couplings between optically induced π-electron rotations and molecular vibrations in a chiral aromatic molecule irradiated by a nonhelical, linearly polarized laser pulse. The results of wave packet dynamics simulation show that the vibrational amplitudes strongly depend on the initial rotation direction, clockwise or counterclockwise, which is controlled by the polarization direction of the incident pulse. This suggests that attosecond π-electron rotations can be observed by spectroscopic detection of femtosecond of femtosecond molecular vibrations [1].

We study the fluorescence emitted from filaments in air using a pump-probe scheme with a femtosecond Ti-sapphire laser. The fluorescence intensities from the first negative band ($B^2\Sigma_u^+ \rightarrow X^2\Sigma_g^+$) and the second positive band ($C^3\Pi_u \rightarrow B^3\Pi_g$) show enhancement and change periodically as a function of the pump-probe time delay. We attribute this phenomenon to the universal yet probably forgotten phenomenon of population trapping of nitrogen molecules in highly excited states together with field-induced alignment of nitrogen molecules followed by revival of the rotational wavepackets. Theoretical calculation of the alignment dynamics of nitrogen molecules is consistent with the experimental data [2].

A main purpose of this work is to show how to employ the inverse Born–Oppenheimer approximation as a basis set to study zero kinetic energy (ZEKE) spectroscopy and the autoionization dynamics of the ZEKE states. The calculations of channel couplings, quantum defects, intensity borrowing, vibrational and rotational autotionizations are demonstrated by using a homonuclear diatomic molecule as an example [3].

Superexcited states (SESs) of oxygen molecules and their neutral dissociation processes have been studied both experimentally and theoretically using intense femtosecond laser. We find that at the laser intensity of approximately 2 x 10^{14} W/cm^2, ultrashort laser pulse causes neutral dissociation of oxygen molecule by way of SESs. The dissociation products are the excited neutral oxygen atoms, which are observed through fluorescence spectroscopy. Laser power dependence of the fluorescence intensity shows that each molecule effectively absorbs an average of ten laser photons. The total energy absorbed is sufficient to stimulate the molecule to many of the SESs. The effect is equivalent to single photon excitation in the extreme-ultraviolet (XUV) region by synchrotron radiation (SR). Morse potential energy curves (PECs) are constructed for the SESs of O_2 molecules. In light of the PECs, predissociation mechanism is proposed for the neutral dissociation. Quasi-classical trajectory (QCT) calculations show that the predissociation time is as short as 100 fs, which is consistent with our experimental measurement using ultrafast pump-probe technique[4].

This work demonstrates a quantitative interpretation of ion desorption in matrix-assisted laser desorption/ionization (MALDI). The theoretical modeling incorporates transition state theory for the desorption of surface ions, assuming chemical and thermal equilibrium in the solid state prior to desorption. It is distinct from conventional models that assume chemical equilibrium in the gas phase. This solid-state thermodynamic interpretation was used to examine the desorption of pure 2,4,6-trihydroxyacetophenone (THAP) and of angiotensin I mixed with THAP. It successfully described the changes in ion yield with the effective temperature under various laser fluence and initial temperature conditions. The analysis also revealed the key role played by ion concentration in the modeling to provide the best fit of the model to observations. On the other hand, divergence of the ion beam with laser fluence was examined using an imaging detection method, and the signal saturation normally seen at high fluence was appropriately reduced by ion focusing. Simplified but deceptive theoretical interpretations were obtained when the analysis was conducted without adequate calibration of the instrument bias [5].

In this work we report a method for controlling electronic localization in a molecular ion, on an attosecond time scale, using a high-intensity laser, based on two different excitation mechanisms. One takes place during ionization, and the other takes place sequentially, following ionization. The electronic excited states of the hydrogen molecular ion are created during ionization by taking the configuration interaction mixing of neutral molecules into account. We detect the ultrafast oscillatory electronic motion between two atoms in a hydrogen molecular ion occurring due to the creation of excited states during the course of ionization [6].

Ⅰ. 3 Discussion

From our experience on quantum control of molecular processes in this project, we found that the commonly used theoretical approach is the solution of the time-dependent electronic and nuclear Schrödinger eqections and that the density matrix method can become a powerful method for studying this type of problems. Since we are very familiar with this approach, we have begun to investigate the quantum control of molecular processes by using the density matrix method.

Ⅰ. 4 Reference

1. M. Kanno, H. Kono, Y. Fujimura and S. H. Lin, Phys. Rev. Lett., 104, 108302(2010) " Nonadiabatic Response Model of Laser-induced Ultrafast π-Electron Rotations in Chiral Aromatic Molecules.
2. A. Azarm, S. Ramakrishma, A. Telebpour, S. Hosseini, Y Teranishi, H. L. Xu, Y. Kamali, J Bernhardt , S. H. Lin, T Seideman and S. L. Chin, J. Phys. B.,At Mol. Opt. Phys. 43, (2010),"Population Trapping and Rotational Revival of N_2 Molecules during Filamemtation of A Femtosecond Laser Pulse in Air".
3. Yi-Hsieh Wang, Y. Teranishi, H. Mineo, S. D. Chao, H. L. Selzle, H. J. Neusser, E. W. Schlag, S. H. Lin, Chemical Physics Letters 486, 104-109(2010). "Theoretical studies of ZEKE spectroscopy and dynamics of high Rydberg states".
4. Di Song, Ali Azarm, Yousef Kamali, Kai Liu, Andong Xia, Yoshiaki Teranishi, Sheng-Hsien Lin, Fanao Kong, and See Leang Chin, J. Phys. Chem. A, 114, 3087-3095 (2010). " Neutral Dissociation of Superexcited Oxygen Molecules in Intense Laser fields".
5. Yin-Hung Lai, Chia-Chen Wang, Sheng-Hsien Lin, Yuan Tseh Lee, and Yi-Sheng Wang, J. Phys. Chem. B, 114,13847-13852 (2010). " Solid-Phase Thermodynamic Interpretation of Ion Desorption in Matrix-Assisted Laser Desorption/Ionization.
6. H. Mineo, Y. Teranishi, S. D. Chao, S. H. Lin, Chemical Physics Letters 499, 45-50 (2010). " Ultrafast electronic motion in hydrogen molecular ions induced by a high power intense laser".

Part Ⅱ Investigations of Photophysics of Organic Solar Cells. 有機太陽能電池光物理之研究

Ⅱ.1 Introduction

A main purpose of this project is to perform the first-principle calculations of internal conversion, abscrption spectra and fluorescence spectra of proto-type molecules for S_0—S_1 and compare the results with experimental ones. The agreement is satisfactory. Another purpose is to examine the anharmonic effect on the photophysical properties of intermediate size molecules and unimolocular dissociation of molecular clusters.

Ⅱ. 2 Results

We have carried out a close examination on the mathematical treatment and the first-principle computations concerning the vibronic transitions between the $S_0{}^1A_1$and the $S_1{}^1A_2$ states of formaldehyde. The simulation of absorption spectrum was reported with peak intensities calculated according to vibronic-coupled transition dipole moments and Franck-Condon factors. The radiative and non-radiative transition rate constants from the excited to the ground states were calculated with formulas based on Fermi's golden rule. It is concluded that our simulated absorption spectrum between 300 and 360 nm, as well as the estimated relaxation rate constants, showed good agreements with experimental reports[7].

The spectra of symmetry-forbidden transitions and internal conversion were investigated in the present work. Temperature dependence was taken into account for the spectra simulation. The vibronic coupling, essential in the two processes, was calculated based on the Herzberg-Teller theory within the Born-Oppenheimer approximation. The approach was employed for the symmetry-forbidden absorption/fluorescence, and internal conversion between 1^1A_{1g} and 1^1B_{2u} states in benzene. Vibrational frequencies, normal coordinates, electronic transition dipole moments, and non-adiabatic coupling matrix elements were obtained by *ab initio* quantum chemical methods. The main peaks, along with the weak peaks, were in good agreement with the observed ones. The rate constant of the $1^1A_{1g} \leftarrow 1^1B_{2u}$ internal conversion was estimated within the order of $10^3 s^{-1}$. This could be regarded as the lower limit (about $4.8 \times 10^3 s^{-1}$) of the internal conversion. It is stressed that the distortion effect was taken into account both in the symmetry-forbidden absorption/fluorescence, and the rate constants of internal conversion in the present work. The distortion effects complicate the spectra and increase the rate constants of internal conversion[8].

Effects of high pressure in a range of up to 1.7 GPa on ultrafast energy relaxation of LDS698 ($C_{19}H_{23}N_2O_4C1$) molecules in solution have experimentally been illustrated by a method of femtosecond time-resolved absorption spectroscopy. The rates of the intramolecular and intermolecular energy relaxations show quite different pressure dependences. The observed results are in good agreement with the theoretical interpretation based on the pressure influences on the molecular energy gaps, the intermolecular H-bond interaction, and the solution viscosity[9].

Investigations on the dissociation kinetics of hydrated protonium ions, $(H_2O)_2\ H^+$ and their deuterated species $(D_2O)_2\ D^+$, are reported based on the harmonic and anharmonic oscillator model using the transition state theory and ab initio calculations. We find that the dissociation of $(H_2O)_2\ H^+$ and $(D_2O)_2\ D^+$ exhibits a distinct threshold behavior due to the existence of activation energies. Moreover, the deviation between the harmonic and anharmonic dissociation rate constants becomes larger in the high energy or temperature range, with the rate constants becoming unreasonably large under the harmonic oscillator model. The isotope effect is found to become more distinct but only in the case of the anharmonic oscillator model. These results show that the anharmonic Rice-Ramsperger-Kassel-Marcus (RRKM) theory can provide a reasonably good description for the dissociation of $(H_2O)_2\ H^+$ and $(D_2O)_2\ D^+$. Furthermore, a theoretical model to demonstrate the principle of vibrational predissociation spectroscopy (VPS) is established from the viewpoint of RRKM theory and applied in determining the experimental conditions and understanding the role of the dissociation rate constant k(E) played in the VPS experiment, using $(H_2O)_2\ H^+$ and $(D_2O)_2\ D^+$ as examples[10].

We have observed rotationally resolved ultrahigh-resolution fluorescence excitation spectra of the 0_0^0 (*a*-type) and 0_0^0 +467cm^{-1} (*b*-type) bands of the $S_2\ {}^1A_2 \leftarrow S_0\ {}^1A_1$ transition of jet-cooled azulene. The observed linewidth is 0.0017cm^{-1}, which corresponds to the lifetime of 3.1 ns in the S_2 state. Zeeman splitting of rotational lines is very small so that intersystem crossing to the triplet state is considered to be very slow. Inertial defect is very small and the molecule is considered to be planar in the S_0 and S_2 states ($C_{2}v$ symmetry). Rotational constants of the S_2 state are almost identical to those of the S_0 state, indicating that geometrical structure is similar in both electronic states. In this case, internal conversion (IC) by vibronic coupling is thought to be inactive. Therefore, the main radiationless transition process in the $S_2\ {}^1A_2$ state of azulene was identified to be IC to the $S_1{}^1B_2$ state. However, this $S_2 \rightarrow S_1$ IC is still slower than that of conventional polycyclic aromatic hydrocarbons. We consider it to be due to the shallower potential energy curve in the $S_1{}^1B_2$ state, which is also responsible for the extraordinarily fast $S_1 \rightarrow S_0$ IC in the isolated azulene molecule [11].

Vibrational level structure in the $S_0{}^1A_g$ and $S_1{}^1B_{3u}$ states of pyrene was investigated through analysis of fluorescence excitation spectra and dispersed fluorescence spectra for single vibronic level excitation in a supersonic jet and through referring to the results of ab initio theoretical calculation. The vibrational energies are very similar in the both states. We found broad spectral feature in the dispersed fluorescence spectrum for single vibronic level excitation with an excess energy of 730 cm^{-1}. This indicates that intramolecular vibrational redistribution efficiently occurs at small amounts of excess energy in the $S_1{}^1B_{3u}$ state of pyrene. We have also observed a rotationally resolved ultrahigh-resolution spectrum of the 0_0^0 band. Rotational constants have been determined and it has been shown that the pyrene molecule is planar in both the S_0 and S_1 states, and that its geometrical structure does not change significantly upon electronic excitation. Broadening of rotational lines with the magnetic field by the Zeeman splitting of M_J levels was very small, indicating that intersystem crossing to the triplet state is minimal. The long fluorescence lifetime indicates that internal conversion to the S_0 state is also slow. We conclude that the similarity of pyrene's molecular structure and potential energy curve in its S_0 and S_1 states is the main cause of the slow radiationless transitions [12].

The dissociation rate constants for hydrogen fluoride dimers are calculated using the YL method, proposed by Yao and Lin (Yao, L.; Mebel, A. M.; Lu, H. F.; Neusser, H. J.; Lin, S. H. J. Phys. Chem. A 2007, 111, 6722). The dividing surface method and RRKM theory are also used to obtain pseudo-transition states and rate constants, respectively. For the dissociation of HF dimers, the anharmonic rate constants are around 3.02 x 10^{10} to 3.46 x 10^{12}s^{-1}, while the harmonic rate constants are in the range of 2.93 x 10^{10} to 1.66 x 10^{13} s^{-1}, at a temperature range of 243-1000 K, for the canonical case. For the microcanonical case, the anharmonic rate constants are in the range of 1.91 x 10^{12} to 1.32 x 10^{13} s^{-1} and the harmonic rate constants are in the range of 1.89 x10^{12} to 4.93 x10^{13} s^{-1}, with a total energy range of 1338-4500 cm^{-1}. Both harmonic and anharmonic rate constants are only comparable to the experimental results 0.5 x 10^{10} s^{-1} and 1 x 10^{11} s^{-1} in an inert gas bath at room temperature. In this case the harmonic and anharmonic rate constants show similar results in this calculation. The results of this work indicate that the YL method is suitable for calculating dissociation rate constants of small flexible HF dimers and the anharmonic effect should be included [13].

Anharmonic effects of the absorption and fluorescence spectra of pyridine molecule are studied and analyzed for the two-low lying singlet excited states $S_1({}^1B_1)$ and $S_2({}^1B_2)$. The complete active space self-consistent field (CASSCF) method is utilized to compute equilibrium geometries and all 27 vibrational normal-mode frequencies for the ground state and the two excited states. The present calculations show that the frequency differences between the ground and two excited states are small for the ten totally symmetric vibrational modes so that the displaced oscillator approximation can be used for spectrum simulations. The Franck-Condon factors within harmonic approximation basically grasp the main features of molecular spectra, but simulated 0-0 transition energy position and spectrum band shapes are not satisfactorily good for $S_1(^1B_1)$ absorption and fluorescence spectra in comparison with experiment observation. As the first-order anharmonic correction added to Franck-Condon factors, both spectrum positions and band shapes can be simultaneously improved for both absorption and fluorescence spectra. It is concluded that the present anharmonic correction produces a significant dynamic shifts for spectrum positions and improves spectrum band shapes as well. The detailed structures of absorption spectrum of $S_2(^1B_2)$ state observed from experiment can be also reproduced with anharmonic Franck-Condon simulation, and these were not shown in the harmonic Franck-Condon simulation with either distorted or Duschinsky effects in the literature[14].

Conformation-dependent properties of $_L$-Phenylalanine in neutral and radical cations have been studied by using density functional theory (DFT) with a new density functional M05-2X, which is applicable to molecular systems with nonconvalent interactions. Adiabatic and vertical ionization energies and charge distributions in the cationic conformers in addition to optimized geometrical structures for both the neutral and the cationic conformers were evaluated. These results were compared with DFT (B3LYP) results. The M05-2X results can explain the correspondence between the observed and predicted conformers without ambiguity. The possibility of conformerization of neutral conformers is indicated from the results of IRC (intrinsic reaction coordinate) profiles [15].

Ⅱ. 3 Discussion

Effect of conical intersections on internal conversion has attracted considerable attention for a number of years. Very recently creditable measurements of the lifetime of the S_2 state of pyrazine have been performed by Suzuki et al (JCP 2010) using the 20fs laser. We are in the process of using the density matrix method to analyze their experimental data and performing the first-principle calculations of this lifetime of pyrazine.

Ⅱ. 4 Reference

7. C. K. Lin, M. C. Li, M. Yamaki, M. Hayashi and S. H. Lin, Phys. Chem. Chem. Phys., 12, 11432 (2010), “A Theoretical Study on the Spectroscopy and Radiative and Non-radiative Relaxation of the $^1A_1-^1A_2$

Transitions of Formaldehyde".

8. J. Li, C. K. Lin, X. Y. Li, C. Y. Zhu and S. H. Lin, Phys. Chem. Chem. Phys., 12,14967(2010). " Symmetry-forbidden Vibronic Spectra and Internal Conversion in Bonzene".

9. B. Liu, C. He, M. Jin, Q.Q. Wang, S. H. Lin and D. Ding, Optics Exp., 18,6863 (2010). " High Pressure Effect on the Ultrafast Energy Relaxation Rate of LD698 in a Solution."

10. Di Song, Hongmei Su, Fan-ao Kong, and Sheng-Hsien Lin, J. Phys. Chem. A, 114,10217-10224(2010). "Anharmonic RRKM Calculation for the Dissociation of $(H_2O)_2H^+$ and Its Deuterated Species $(D_2O)_2D^{+}$"

11. Yosuke Semba, Kazuto Yoshida, Shunji Hasahara, Chi-King Ni, Yen-Chu Hsu, Sheng Hsien Lin, Yasuhiro Ohshima, and Masaaki Baba, The Journal of Chemical Physics 131,024303(2009)." Rotationally resolved ultrahigh-resolution laser spectroscopy of the S_2 $^1A_1 \leftarrow S_0$ $^1A_1$ transition of azulene".

12. Masaaki Baba, Motohisa Saitoh, Yasuyuki Kowaka, Kunio Taguma, Kazuto Yoshida, Yosuke Semba, Shunji Kasahara, Takaya Yamanaka, Yasuhiro Ohshima, Yen-chu Hsu, and Sheng Hsien Lin, The Journal of Chemical Physics 131,224318(2009). "Vibrational and rotational structure and excited-state dynamics of pyrene".

13. L. Yao, A.M. Mebel, S. H. Lin, J. Phys. Chem. A *113,* 14664-14669 (2009). " Dissociation Rate Constant of the Hydrogen Fluoride Dimer by the ab Initio Anharmonic RRKM Theory".

14. Huan Wang, Chaoyuan Zhu, Jian-Guo Yu, and Sheng Hsien Lin, J. Phys. Chem. A 113,14407-14414(2009). "Anharmonic Franck-Condon Simulation of the Absorption and Fluorescence Spectra for the Low-Lying S_1 and S_2 Excited States of Pyridine".

15. K. Y. Baek, M. Hayashi, Y. Fujimura, S. H. Lin, and S. K. Kim, J. Phys. Chem. A 114, 7583-7589 (2010). "Investigation of Conformation-Dependent Properties of $_{\mathrm{L}}$-Phenylalanine in Neutral and Radical Cations by Using a Density Functional Taking into Account Noncovalent Interactions".

國科會補助計畫衍生研發成果推廣資料表

日期:2010/12/25

國科會補助計畫	計畫名稱: 子計畫一：飛秒超強光雷射化學之研究；子計畫二：有機太陽能電池光物理之研究
	計畫主持人: 林聖賢
	計畫編號: 98-2113-M-009-009-　　學門領域: 物理化學

無研發成果推廣資料

98 年度專題研究計畫研究成果彙整表

計畫主持人：林聖賢	**計畫編號：**98-2113-M-009-009-
計畫名稱：子計畫一：飛秒超強光雷射化學之研究；子計畫二：有機太陽能電池光物理之研究	

成果項目			量化			單位	備註（質化說明：如數個計畫共同成果、成果列為該期刊之封面故事...等）
			實際已達成數（被接受或已發表）	預期總達成數(含實際已達成數)	本計畫實際貢獻百分比		
國內	論文著作	期刊論文	0	0	100%	篇	
		研究報告/技術報告	0	0	100%		
		研討會論文	0	0	100%		
		專書	0	0	100%		
	專利	申請中件數	0	0	100%	件	
		已獲得件數	0	0	100%		
	技術移轉	件數	0	0	100%	件	
		權利金	0	0	100%	千元	
	參與計畫人力（本國籍）	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%		
國外	論文著作	期刊論文	0	0	100%	篇	
		研究報告/技術報告	0	0	100%		
		研討會論文	0	0	100%		
		專書	0	0	100%	章/本	
	專利	申請中件數	0	0	100%	件	
		已獲得件數	0	0	100%		
	技術移轉	件數	0	0	100%	件	
		權利金	0	0	100%	千元	
	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）