



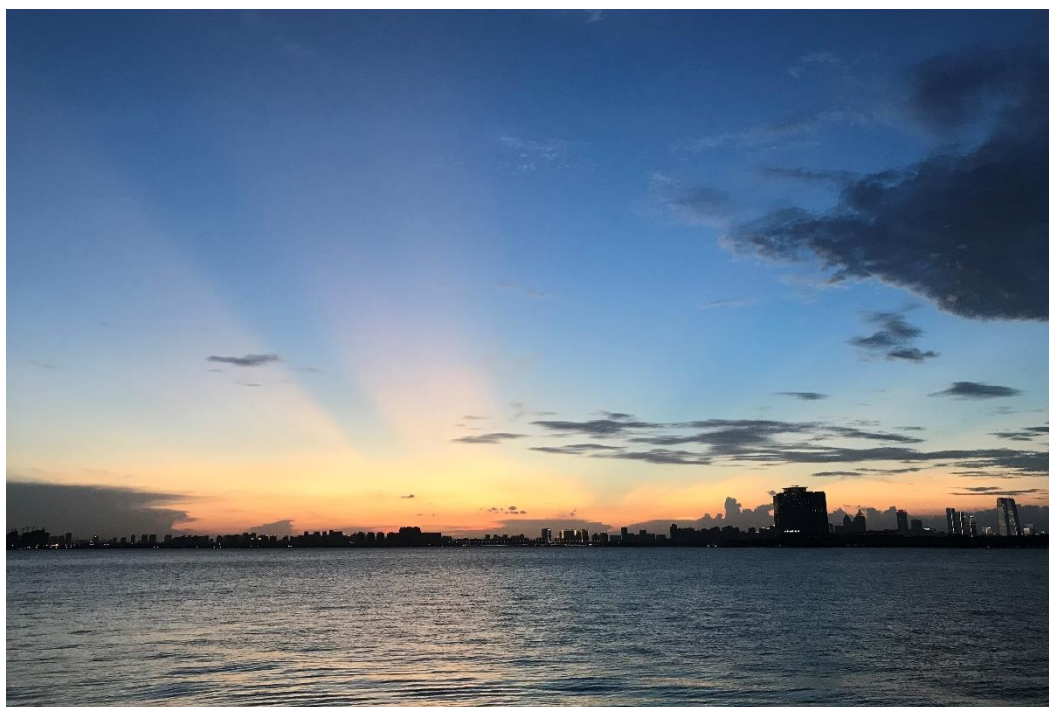
会议简介

由中国化学会主办、复旦大学和苏州大学承办的第十六届全国化学动力学会议，定于2019年10月11-14日在江苏省苏州市相城区阳澄湖畔举行。此次会议诚邀从事化学动力学研究的国内外专家学者参加，展示化学动力学领域中的最新成果，分析当前国际研究的前沿和热点，主要围绕以下5个方向开展学术交流：1. 气相、凝聚态和界面化学动力学；2. 离子、自由基和团簇化学动力学；3. 动力学光谱、激光化学和光化学动力学；4. 化学反应动力学理论、实验新方法；5. 生物分子化学动力学。

我们热忱欢迎各位同行参加，并祝愿大家取得丰硕的交流成果，共同促进中国化学动力学的发展。

第十六届全国化学动力学会议筹备委员会

2019年10月10日



 会议组织

会议筹备组 (排名不分先后)

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 交通指南**苏州市在水一方大酒店交通指南**

地点：苏州市相城区尊园路 1 号

1. 苏州高铁北站：

- 乘快线 7 号到“相城区行政中心南”，步行 770 米到达酒店
- 乘地铁 2 号线到“阳澄湖中路”（1 出口），步行至“纪元路采莲路东站”公交站，乘 881 路到“澄阳路南”，步行 530 米到达酒店
- 乘的士约需 25 元，全程约 21 分钟到达酒店

2. 苏州站：

- 乘 83 路到“中翔家电小商品市场”，步行 890 米到达酒店
- 乘地铁 2 号线到“阳澄湖中路”（1 出口），步行至“纪元路采莲路东站”公交站，乘 881 路到“澄阳路南”，步行 530 米到达酒店
- 乘的士约需 23 元，全程约 20 分钟到达酒店

3. 上海虹桥国际机场：

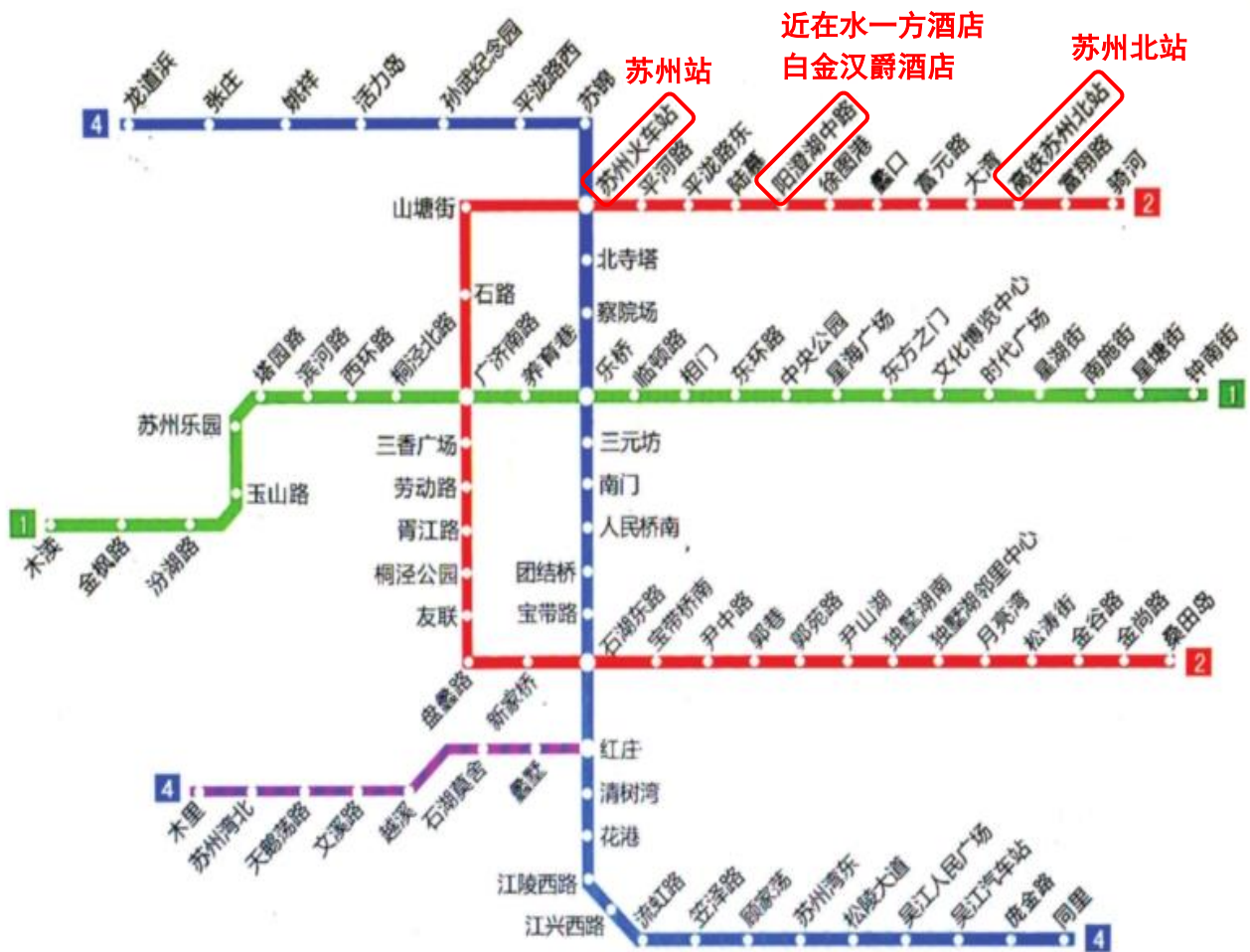
- 乘高铁到“苏州站”，全程约 35 分钟
- 乘高铁到“苏州高铁北站”，全程约 40 分钟

4. 无锡苏南硕放国际机场：

- 乘的士到“在水一方大酒店”，约需 104 元，全程约 34 分钟到达酒店

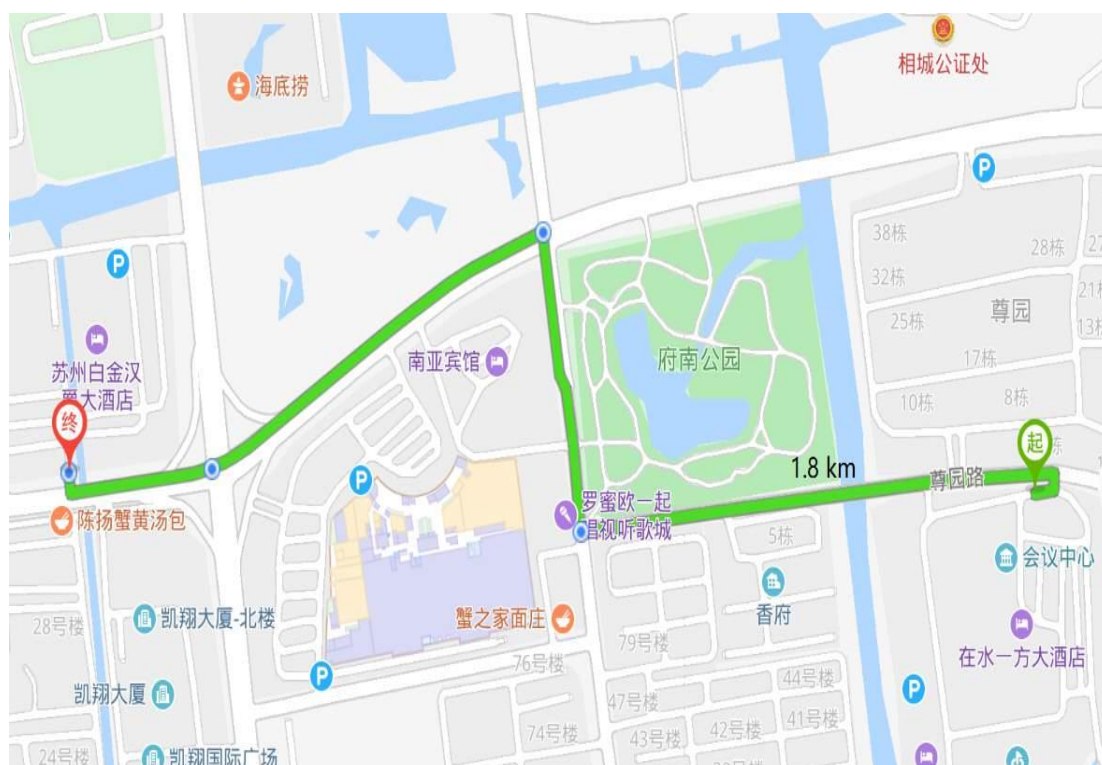
交通指南

苏州轨道交通 Suzhou Rail Transit



 交通指南

会议酒店地点示意图



苏州白金汉爵酒店 ←→ 在水一方酒店

步行路线：全程约 1.8 公里，步行约 16 分钟。

打车路线：距离 1.8 公里，打车约 10 元，全程约 6 分钟。



会议摘要

K1 Probing Geometric Phase Effect in Chemical Reaction

杨学明

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It was long predicted theoretically that geometric phase effect could have a significant effect in the dynamics of chemical reactions with conical intersections. However, experimental observation of such effect proves to be extremely difficult and fruitless. Recently, a high resolution crossed beams imaging apparatus has been developed, geometric phase effect in the $H+HD\rightarrow H_2+D$ reaction was observed clearly at collision energy above the conical intersection of this reaction using the high resolution threshold ionization - imaging technique. In addition, we have also detected experimental evidence of geometric phase effect, through energy dependent quantum-state-resolved DCS oscillations due to quantum interference between topological pathways, at collision energies significantly lower than the conical intersection energy using high resolution H-atom Rydberg tagging crossed molecular beams method. These new experiments in combination with accurate quantum dynamics calculations allows us to probe and understand this interesting dynamics effect in chemical reaction at the most fundamental level.

K2**Water Effects on Atmospheric Reactions****Joseph S. Francisco**

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Water has a very significant impact on the processes that occur in the Earth's atmosphere. Water is one of the most abundant resources in our atmosphere and, because of its ability to be both a hydrogen bond donor and acceptor, it can form very stable complexes. The formation of these complexes can dramatically affect the chemistry in the atmosphere, including heterogeneous removal and alteration of the photochemical properties of the atmospheric species, the formation of water droplets and aerosol particles, as well as the participation of these complexes in chemical reactions. This talk will provide a comprehensive look at both the experimental and theoretical investigations of water vapor effects on gas phase reactions, with an emphasis on those pertinent to the atmosphere. A goal of the talk is to provide an understanding of the fundamental concepts that lead to potential water effects, imparting a framework to realize the global effects of water in our atmosphere.



K3

非绝热动力学过程的理论计算模拟

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Born-Oppenheimer (B-O) 近似是化学、物理以及生物学科的重要基石。然而, 绝大多数光诱导的化学、生物以及材料光响应过程是非平衡、非绝热的, B-O近似常常失效。围绕光诱导化学及生物过程的关键理论问题: 势能面交叉和非绝热动力学, 主要结合报告人课题组有关非绝热动力学过程的理论工作, 简单回顾非绝热动力学的研究背景, 重点交流相关理论和计算模拟的进展, 也将探讨可能的突破方向。

关键词: 非绝热效应; 动力学模拟; 光化学反应

K4

表面吸附体系的自旋输运和调控

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自旋电子学利用电子自旋进行信息的传递、处理与存储，具有目前传统微电子学器件无法比拟的优势，例如运算速度快，能耗低等，因而成为近年来人们研究的热点。在原子或分子尺度上实现对自旋态的测量和调控是我们面临的一个重要科学挑战，扫描隧道电子显微镜（STM）的发明为我们提供了研究手段，吸附体系的 Kondo 效应提供了研究对象。本报告针对 STM 对表面吸附磁性原子和分子体系的输运测量及操纵，系统发展了基于第一性原理的 Kondo 效应的谱学计算方法，为多种表面吸附体系的自旋输运和调控提供理论机理和解释。

翁羽翔

中国科学院物理研究所 软物质物理院重点实验室

生物量子效应是近年来备受关注的研究领域，光合作用是研究生物量子效应的优势系统。光合作用原初吸能、传能超快过程是由镶嵌于光合膜上的天线膜蛋白实现的，光合膜蛋白包含捕光色素分子和固定色素分子的蛋白质骨架。在漫长的演化过程中，相应的蛋白进化出对色素分子某些量子态的静态及动态的调控，以实现适应环境的特殊功能。具体是光合系统通过对色素分子的选择及不同聚集态的调控，从而实现具有不同性能的量子态，而蛋白质通过结构变化进一步调节上述量子态的性质。本报告以两个典型的系统，揭示光合系统动态调节过程所展示的生物量子效应。

(1) 高等植物捕光天线实现高效捕光和激发能耗散的蛋白质开关机制。

在自然环境中，太阳光的辐照强度短时间内可呈现十几倍的差异。为此高等植物进化出非常精巧的调节机制，从而最大限度地优化光合作用效率并避免光损伤。光合系统不仅要在低光照条件下开启高效捕光的功能，将激发能高效地传给反应中心进行后续的光合作用；还要在高光条件下将激发能通过热的形式耗散掉，从而切断能量传递通路，避免过量的光能所造成的辐射损伤，实现其光保护功能。我们通过超快光谱、纳秒脉冲升温-时间分辨中红外光谱及分子动力学模拟研究，揭示光合膜蛋白动态结构是如何与光合膜的力学性质相耦合，促成光合系统对外界光强变化的主动相应，协同完成对传能效率的优化以及光保护功能的切换。

(2) 合细菌外周捕光天线膜蛋白结构与光合膜囊泡最优化尺寸

在光合细菌的生长过程中，光合膜囊泡的尺寸随外界光强的变化而变化。在低光照条件下，其直径约为 50nm。光合膜内光合细菌捕光天线色素蛋白复合体 LH2 晶体结构数据表明其具有 C9 对称的圆环状结构。叶绿素分子组成两个色素环，其中一个色素环由单体叶绿素分子构成，吸收光谱位于 800nm；另一个由 9 对叶绿素二聚体分子构成，吸收光谱在 850nm。我们应用小角 X-射线散射方法首次从结构学给出溶液中 LH2 结构畸变的实验证据；激子理论预测，LH2 结构发生畸变后，激子态寿命变短。由于光合膜的弯曲作用，可能会引起 LH2 在光合膜上的椭圆畸变，导致传能效率降低。我们通过将 LH2 与一系列直径不等的 SiO₂ 纳米粒子进行组装，模拟 LH2 在囊泡上的结构畸变，揭示蛋白质曲率（光合膜）对 LH2 量子态的调控，从而实现最优化能量的捕获及传递。为此我们应用纳米晶@SiO₂ 核壳结构对共振拉曼增强效应，证明了 LH2 和 SiO₂ 纳米的成功组装；首次实验定量测定了 SiO₂ 表面电荷与密度与粒径的依赖关系；从量子力学的角度阐明辐射跃迁与非辐射跃迁的关系，并通过实验证实；实验确定的通过 LH2 量子效应确定的优化曲率与生物体观测结果相符合。

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K6 Coupling of Methane and Carbon Dioxide by Gas-Phase Ions

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Methane (CH₄) and Carbon dioxide (CO₂) are two abundantly available carbon-based feedstocks. Coupling of CH₄ with CO₂ to form value-added products such as HCHO, CH₃OH, and C₂ compounds are very important research topic. However, both CH₄ and CO₂ molecules are thermodynamically very stable and kinetically inert. It is difficult to activate either of the molecules. By using mass spectrometry based techniques and state-of-the-art quantum chemistry calculations, the reactions of gas-phase ions with CH₄ and CO₂ have been extensively studied to understand the mechanisms of CH₄ activation [1] and CO₂ activation [2] separately, while the ions to mediate the coupling reaction have been rarely identified [3]. This talk will discuss a few oxide and boride species (see one example in Fig. 1) that have been very recently characterized to be able to mediate the coupling of CH₄ and CO₂ in the gas phase.

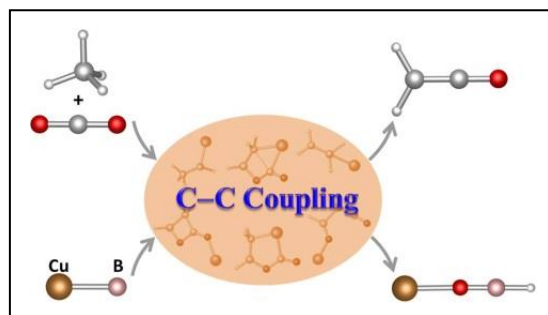


Fig. 1 The C-C coupling of CH₄ and CO₂ by CuB⁺ ions (from Ref. [4]).

Keywords: ion-molecule reactions; C-C coupling; mass spectrometry; quantum chemistry calculations; boride species

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K7 四链体核酸及光活化核酸分子的化学反应动力学研究：从纳秒到飞秒

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核酸是以核苷酸为基本组成单位的生物信息大分子，具有复杂的结构和重要的生物功能。除了五种核酸碱基（ATGCU）以及传统的双链 DNA 结构之外，生命的密码本还存在有化学修饰的碱基，更多在调控生命过程中起到作用的新颖的核酸二级结构被发现。我们利用纳秒、飞秒的时间分辨光谱技术，研究了四链体 DNA（G-四链体、i-motif 等）以及硫代、卤代碱基等光活化核酸分子的光化学和光物理过程的动力学机理。比如，我们研究了胞嘧啶 C 碱基氧化损伤的重要中间体：胞嘧啶自由基阳离子（ $C^{+\bullet}$ ），在一类重要的非 B 型 DNA i-motif 结构中的基元反应途径。有趣的是，我们观察到 $C^{+\bullet}$ 的反应途径在 i-motif 结构与自由碱基 dC 截然不同，在自由碱基中主要是脱质子的互变异构反应，而在 i-motif 中主要表现为 $C^{+\bullet}$ 水合生成 $C(5OH)^{\bullet}$ 和 $C(6OH)^{\bullet}$ 的光谱特征。通过进一步的 pH 依赖实验，单链 DNA 对照实验，以及银离子调节形成的 i-motif DNA 对照实验，我们揭示了结构相关的反应机理。不仅揭示了氢键结构微环境对 $C^{+\bullet}$ 基元反应途径的重要影响，尤其对于 i-motif DNA，我们的结果表明 $C^{+\bullet}$ 水合以及水合产生的 $C(5OH)^{\bullet}$ 和 $C(6OH)^{\bullet}$ 会引发一系列次级反应进而破坏 i-motif 的稳定性及结构，而 i-motif DNA 发挥其生物功能是高度依赖于其四链结构的。另外，我们利用 Ru-dppz 配合物的光开关性质，将其与 G-四链体 DNA 结合，通过纳秒发光动力学以及暗态过程的飞秒瞬态吸收光谱测量，探测四链体结构微环境的水的特性，发现四链体 loop 区域具有部分疏水、部分亲水的特性。

K8

分子真空紫外光化学动力学研究

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分子光化学动力学研究在过去几十年取得了很大的进展, 几乎所有小分子在紫外波段的光化学都有研究报道, 而在真空紫外波段, 受限于高亮度可调谐的真空紫外光源的缺乏, 分子在这一波段的研究无论是国内还是国际都比较稀少。而恰恰宇宙诞生早期最重要的一些分子, 比如 H_2 , CO , H_2O , CO_2 , CH_4 等分子的光化学都位于真空紫外区, 对于这些分子的光化学应该怎么去研究? 过去十年来, 我们实验室通过四波混频技术产生了可调的真空紫外光源并与高分辨的里德堡氢原子技术相结合, 研究了水分子最低四个电子激发态的光解动力学。最近两年来, 我们搭建了基于大连极紫外自由电子激光的分子光化学实验站, 并进行了系统的分子真空紫外光化学的研究工作。这次报告主要介绍大连极紫外自由电子激光在水分子和二氧化硫分子高电子激发态的光解动力学研究。

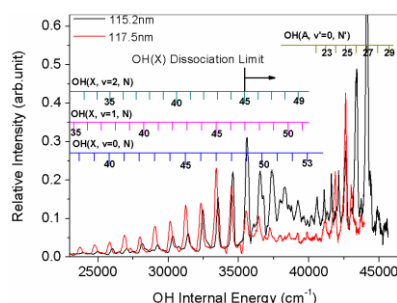


Figure 1: Internal energy spectra of the OH products from photodissociation of H_2O at 117.5 nm (red) and 115.2 nm (black), obtained from H atom TOF spectra recorded with the detection axis parallel to the photolysis laser polarization.

关键词: 真空紫外; 极紫外自由电子激光; 里德堡氢原子时间飞行谱

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K10

双原子分子间传能动力学的理论研究

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分子间碰撞是气相条件中重要的物理化学过程，研究分子间传能动力学在大气化学、激光化学、星际化学等领域都有广泛的应用价值。氟化氢（HF）分子是化学激光器中的工作介质，HF与激光器中其他分子的振动弛豫速率常数是发展化学激光器的关键参数。在实验上，要精确测定转动态分辨的传能速率常数仍有一定困难。

近年来，我们发展了“包含最邻近科里奥利耦合的态耦合近似”（CSA-NNCC）方法，并证明该方法相比于严格的非含时动力学方法，计算误差较小但大大节省了计算量。并构建了H₂-HF和HF-HF体系全维高精度从头算势能面，开展了这两个体系转动传能、振转传能动力学计算。纯转动的H₂-HF体系传能积分截面、速率常数的计算结果与其他理论值对照良好。振动传能方面，对于HF分子处于振动基态和振动激发态的H₂-HF体系的V-V传能速率常数和HF-HF体系的V-T传能速率常数，计算结果均与实验值相符良好。

除了与实验值对比，理论计算能够为我们提供更详细的微观反应机制和对化学物理过程的理解。传能反应一般遵守“内能守恒”和“内角动量守恒”定律，即对于给定的初态，传能以那些与初态内能相近、内角动量与初态一致的传能末态为主导。我们发现H₂-HF振动弛豫体系的规律与传能一般规律“内能守恒”定律相符很好，但HF-HF体系却与该定律有所偏差。我们进一步的计算证明这是由于HF-HF的较深的范德华深势阱、反应中间复合物(HF)₂寿命长等因素造成的。这些研究为深入理解分子间传能动力学迈出了重要一步。

关键词： 非弹性散射；化学激光；能量传递；速率常数

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K11 Proton Transfer Reaction Dynamics in Condensed Phases: Quantum Effects Using the Reduced Quantum Dynamics Approach

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The non-perturbative hierarchical equations of motion (HEOM) method has developed into an important tool to simulate quantum dynamics in condensed phase. I will present its applications to studies of quantum effects in proton transfer (PT) reactions using model systems: (1) Transition from coherent dynamics to rate dynamics for a double-well model, and the observation of non-Kramers behavior due to quantum tunneling. (2) Effects of the rate promoting vibrational mode, which increases the rate constants and decrease the kinetic isotope effect. (3) A mixed quantum-classical description of the PT dynamics, where the proton degrees of freedom is quantized, while the other degrees of freedom are treated classically. The hydride transfer reaction in DHFR is also mapped into a double-well/harmonic bath model, and studied using the mixed quantum-classical approach. (4) Quantum effects in photo-induced proton coupled electron transfer reactions, where the effect of vibrational relaxation becomes important.

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K12

复杂分子体系的激发态溶剂化过程研究

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绝大多数光化学反应大都是在激发态过程中发生的。在激发态过程的光化学反应中，存在大量的中间态过程，理解这些中间态的结构与性质，是理解化学反应的关键。传统的表征手段，如质谱、红外和 Raman、X 射线衍射等技术，由于自身的限制对光化学的激发态过程中的很多重要的化学过程的探测有极大的局限性。特别是对那些瞬态中间态的演化动力学及其结构的探测非常困难。该报告将简单介绍我们实验室为探测光化学反应激发态过程的演化而研制和发展的飞秒时间分辨光谱探测方法的基本原理和技术方法。重点介绍利用这些技术开展的关于激发态“暗态”过程的调控和探测的研究进展。

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K13 Cavity-enhanced Spectroscopy of Molecules with Unprecedented Precision

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Line positions are the most frequently referenced information obtained from molecular spectroscopy. However, the accuracy of most line positions in the near infrared is limited to 10^{-3} - 10^{-4} cm^{-1} due to the weakness of the lines as well as Doppler broadening. Spectroscopy techniques utilizing high-finesse cavities, including cavity enhanced absorption spectroscopy (CEAS), cavity ring-down spectroscopy (CRDS), and the noise-immune cavity-enhanced optical heterodyne modulation spectroscopy (NICE-OHMS), combined with optical frequency combs, allow us to determine the positions of weak molecular overtone transitions from saturation spectra with unprecedented accuracy [1]. For demonstration, we determined a few CO line positions at 1.6 μm with sub-kHz accuracy (10^{-8}cm^{-1}) [2]. The method was applied to determine the position of an overtone line of HD at 1.4 μm , towards a determination of the proton-to-electron mass ratio [3]. We also developed a cavity-assisted speed-selective double resonance spectroscopy (CASS-DR) technique by coupling two single-frequency lasers into one cavity. The technique was applied to detect Doppler-free DR spectrum of a high overtone band of CO_2 which is symmetry-forbidden for one-photon transition.

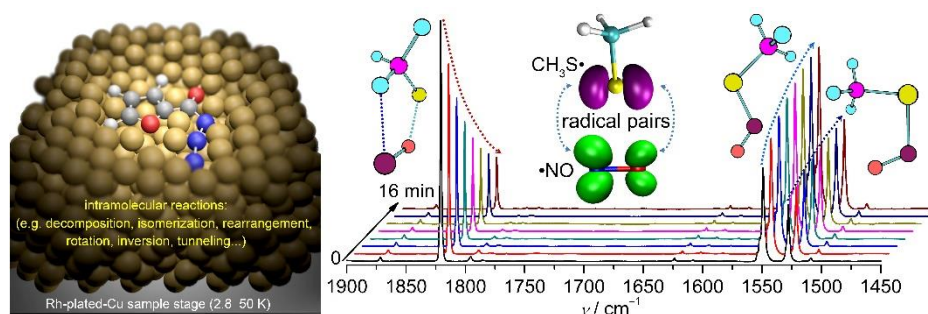
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一直以来, 低温基质隔离光谱(matrix-isolation spectroscopy)被广泛用于不稳定物种如原子、自由基和活泼中间体的原位探测和光化学反应过程的跟踪。该方法主要采用化学较为惰性的气体分子如 Ne、Ar、Kr、N₂ 等为介质, 在极低温 (<40 K) 条件下实现固体基质中不稳定物种的高度分散与冷却, 使其难以发生分子内或分子间的反应, 从而实现室温下瞬态中间体的稳定存在并被光谱探测。相比原位光谱探测, 在极低温惰性基质中研究分子的动力学转化则较为少见。近期, 我们采用低温基质隔离红外光谱, 对几类典型的低能垒过程 (<2 kcal/mol) 即链状共轭多烯自由基的构象转化 (*N*-inversion)^[1]、低价磷的光氧化 (photooxidation)^[2]、以及生物化学过程中重要的自由基对 (radical-pair) 的复合^[3]开展了动力学过程跟踪。结合高精度理论计算对系列新颖瞬态物种进行指纹光谱识别, 发现了同位素交换现象以及获取了相关的动力学参数。


关键词: 低温基质隔离; 红外光谱; 自由基

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K15

F+H₂O/CHD₃ 反应共振态的理论研究张东辉

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2000年，刘国平等人首次在 $F+HD \rightarrow HF+D$ 反应积分截面随反应能变化的曲线上观察到一个有反应共振态所引起的明显台阶，证实了化学反应中确实存在共振态。近些年来，随着实验与理论研究的逐步深入， $F+H_2/HD$ 中的反应共振态得到了彻底的揭示，极大提高了我们对反应共振态的认识。2004年，刘国平等人还在 $F+CHD_3$ 反应中有观测到共振态迹象。2014年郭华、Continetti等人在 FH_2O 负离子光电子谱研究中发现了束缚在 $HF-OH$ 范德华势阱中的共振态。最近，我们构造了 $F+H_2O/CH_4$ 反应高精度的势能面，并在这些势能面上开展了量子动力学研究。我们的计算表明这两个反应在低碰撞能下都存在反应共振态，其中 $F+CHD_3$ 反应共振态机制和 $F+H_2$ 反应一样，都是束缚在主要由化学键软化所引起的产物 $HF(v=3)$ 振动绝热势阱中，而 $F+H_2O$ 反应共振态则是束缚在产物 $HF(v=2)-OH$ 范德华势阱中。



K16

On Scientific Creativity

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This talk is not about the recent finding of my works, rather on some personal thoughts about scientific research. In recent years, “creativity” is becoming a buzz word and has been repeatedly emphasized and sometimes debated in many disciplines. Clearly, it is a vague concept that different people in different fields may view differently. But, as a scientist or a physical chemist, let us get back to basics and ask ourselves: What is scientific creativity? How to make a sound judgement about a scientific project or finding? Can we foster the scientific creativity by ourselves? ... etc. Those are the questions that I would like to address and share my opinions with you in this talk.

11

单个体电化学分析

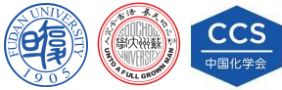
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长期以来，分析化学停留在样本检测的平均信号获取水平，无法识别单个实体间的差异性，而在复杂体系中，结构、组成、性质偏离均值的个体往往具有重要的功能。电分析化学在纳米材料和纳米尺度系统的研究应用中获得新生。单个体电分析化学（Single entity electrochemistry）为认识纳米尺度的电化学反应提供了新途径，为理解复杂体系的电化学反应提供了自下而上的研究方法。

发展高通量、原位、高时空分辨的单个体分析新原理和新方法，将为认识复杂体系，特别是生命体系中物质变化和能量转移过程提供新的工具，将推动了分析化学向极限检测方向发展。



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秒激光具有超短的脉冲宽度和超高的峰值功率，它和气相原子分子相互作用是一种极端非线性过程，能够辐射能量覆盖太赫兹-可见-真空紫外-软X射线波段的光子，为超快可调谐光源的产生提供了重要手段。我们在北京大学建立了原子分子强场物理实验平台，通过对飞秒激光与原子分子相互作用产物光子、电子、离子进行测量，深入研究了飞秒激光和原子分子相互作用机理[1-2]。本报告将介绍我们在飞秒激光与气体相互作用的超快光源产生及应用方面最新研究进展，分为两个部分内容：1) 基于飞秒激光和原子分子相互作用的高次谐波技术，我们在实验室建立了两台台式化超快真空紫外光源。该光源分别与速度成像谱仪和光电子显微镜结合，开展激光驱动的原于分子以及微纳结构的光电子动力学研究。2) 氮气分子离子激光由于在大气远程探测领域有重要的应用潜力而备受关注。我们利用波长800纳米飞秒激光和氮气分子相互作用，通过注入不同波长的种子光或/和控制光，对氮气分子离子激光的物理本质以及产生条件进行了深入研究[3-7]，为氮气分子离子激光优化提供指导。

关键词：高次谐波；光电子显微镜；空气激光；超荧光

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13 Ultrafast Dynamics in Methylated Cytosine and Its Derivatives

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DNA methylation is a stable epigenetic mark that has an important role in gene regulation. DNA methylation in the form of 5-methylcytosine (5mC) can be actively reversed to unmodified cytosine (C) through TET dioxygenase-mediated oxidation of 5mC to 5-hydroxymethylcytosine (5hmC), 5-formylcytosine (5fC) and 5-carboxylcytosine (5caC). Thus, 5-methylcytosine is often referred to “the fifth base of DNA”. A comprehensive understanding of the electronic excited state relaxation in cytosine and its methylated derivatives is crucial for revealing UV-induced photodamage to the biological genome. We used femtosecond time-resolved spectroscopy to comprehensively study the excited state dynamics of 5mC, 5hmC, 5fC and 5caC in solution. Two distinct nonradiative decay channels were directly observed in 5mC and 5hmC singlet states while long-lived triplet state was seen in 5fC but not in 5caC. Potential double proton transfer were also observed in 5hmC, 5fC and 5caC.



14 Forward and Backward Stochastic Schrödinger Equations and Their Applications to Carrier Quantum Dynamics and Spectra in Organic Materials

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The carriers in organic materials commonly follow hopping-type motions because of strong carrier-phonon interactions. However, they can also present a band-like behavior in well-performed organic crystals or hybrid inorganic-organic materials. Therefore, their dynamics should be described by a unified method covering from band-like to hopping-type motions. Development of such a method for large systems is also one of significant tasks for theoretical chemistry and still meets a great challenge. Focusing on this problem, we have proposed a time-dependent wavepacket diffusion method. In the method, the effects of carrier-phonon interaction and inter- or intra-molecular electronic couplings are considered as the dynamical fluctuations on carrier dynamics. Based on this concept, we have further proposed a rigorous hierarchy of stochastic Schrödinger equation, and the relationship between two approaches are built. We also present how to combine electronic structure calculations with these quantum dynamics methods to reveal the carrier dynamics in realistic organic semiconductors, such as exciton energy relaxation, singlet fission and 2D spectra.

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溶液体系动力学振动光谱的理论模拟

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Terahertz-frequency collective vibrational modes of the protein-ligand complexes may guide the system to walk along the proper free energy pathway, therefore facilitate certain biological function. However, the molecular mechanism of how these terahertz modes efficiently mediate the protein-ligand binding and biochemical reactions in general remains elusive, since considerable variation in the nature of such changes has been observed using different tools on different protein-ligand complexes. Further, related experiments are difficult to carry out and interpret. Femtosecond optical Kerr-effect (OKE) spectroscopy, as one of the most efficient and powerful spectroscopic tools for detecting the slow solution dynamics, is sensitive to molecular structural dynamics appear in the terahertz region. Interpreting the sophisticated solution spectra can, in general, largely benefit from theoretical modeling. Due to the size and complexity of protein-ligand aqueous solution system, however, modeling of their OKE signals were considered as not feasible. We herein present the first theoretical modeling work of the OKE signals for a lysozyme-NAG3 aqueous solution system based on the molecular dynamics simulations. The system polarizability is calculated on-the-fly using an analytical expression instead of a dipole-induce-dipole self-consistent treatment, which significantly reduces the computing cost and makes the simulation possible. Further analysis of the simulation results indicates that the apparent blue shift of OKE peak at ~1 Thz is created by a stiffening of ligand due to its binding to lysozyme and a softening of protein domains adjacent to the ligand molecule.



I6 Simultaneous Attenuation of Both Self-Interaction Error and Nondynamic Correlation Error in Density Functional Theory: A Spin-pair Distinctive Adiabatic-Connection Approximation

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We present a spin-pair distinctive algorithm in the context of adiabatic-connection fluctuation-dissipation (ACFD) theorem[1], which enables to quantify the self-interaction error (SIE) and the nondynamic/strong correlation error (NCE) in the direct random-phase approximation (dRPA)[2]. Using this knowledge, we propose a spin-component scaled dRPA (scsRPA) correlation model with simultaneous attenuation of both the SIE and the NCE. Along with the exact exchange, scsRPA is shown to present a comprehensive improvement over dRPA, as well as the well-established PBE and PBE0 functionals, for bonding energies of pronounced multi-reference characters and transition-metal complexes of strongly correlated systems, while consistently provide an accurate description for reaction energies, reaction barriers, and non-covalent bond interactions of weakly correlated systems.

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Biography

Dr. Igor Ying Zhang obtained his PhD degree in Chemistry from Xiamen University, China (2010) and KTH Royal institute of technology, Sweden (2011). In 2012, he joined the Fritz Haber Institute (FHI) Berlin, Germany with a Max-Planck fellowship and was then promoted to be a group leader soon. In March 2018, he moved to Department of Chemistry, Fudan University as an awardee of “the Recruitment Program for Young Professionals”.

Dr. Igor Ying Zhang’s research focuses on the development of advanced first-principle electronic-structure methods towards predictive accuracy for molecules and materials. He is authored and co-authored 40 peer-reviewed papers and one Springer book with over 2600 citations and an H-index of 22 (Google Scholar, Nov. 2019).

17 Recent Development of State-to-state Quantum Reactive Scattering

Theory

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对于理论化学动力学研究来说，发展精确高效的理论计算方法，从来都是十分必要的，尤其对于采用量子动力学原理计算态-态分辨的反应散射过程而言。量子反应动力学计算量大，而对于复杂的态-态动力学过程来说，量子波包方法往往存在所谓的“坐标”问题，很难实现高效率的计算。在过去这些年，我们发展了一系列方法，试图克服态-态量子波包动力学计算中的“坐标”问题。最近我们发展了超球坐标和雅科比坐标混合的IARD方法，首次成功克服了所谓的“坐标”问题，大大提高了态-态量子波包方法的计算效率。在本报告中，我们将对相关工作详细展开讨论。

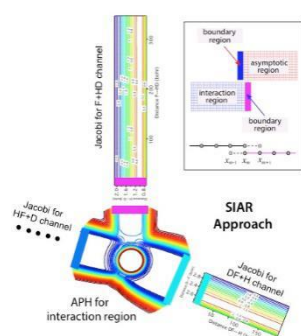
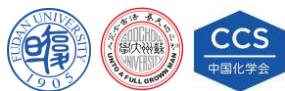


Fig 1. IARD scheme for a state-to-state calculation.

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18 A New Perspective for Nonadiabatic Dynamics with Phase Space

Mapping Models

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Based on the recently developed unified theoretical framework, we propose a new perspective for studying nonadiabatic dynamics with classical mapping models (CMMs) of the coupled multi-state Hamiltonian onto the Cartesian phase space. CMMs treat the underlying electronic state degrees of freedom classically with a simple physical population constraint while employing the linearized semiclassical initial value representation to describe the nuclear degrees of freedom. We have tested various benchmark condensed phase models where numerically exact results are available, which range from finite temperature to more challenging zero temperature, from adiabatic to nonadiabatic domains, and from weak to strong system-bath coupling regions. CMMs demonstrate overall reasonably accurate dynamics behaviors in comparison to exact results even in the asymptotic long time limit for various spin-boson models and site-exciton models. Further investigation of the strategy used in CMMs may lead to practically useful approaches to study nonadiabatic processes in realistic molecular systems in condensed phase.

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Biography

Jian Liu obtained B.S. (2000) from the University of Science & Technology of China and then Ph.D. (2005) from the University of Illinois at Urbana-Champaign. He worked as a postdoctoral fellow at the University of California, Berkeley (2005-2011) and then as a research associate at Stanford University (2011-2012), before he was appointed Associate Professor at the College of Chemistry and Molecular Engineering, Peking University (2012-present). His research interests has focused on the development of theories and methodologies of quantum/semiclassical dynamics and quantum statistics for complex/large molecular systems. Liu was a recipient of the American Chemical Society Physical Chemistry Division Postdoctoral Research Award (2012), the Chinese National "Thousand Young Talents Program" fellowship (2012), the Chinese Chemical Society Tang Au-Qing Youth Award on Theoretical Chemistry (2015), the 2018 QSCP Promising Scientist Prize of CMOA (Centre de Mécanique Ondulatoire Appliquée), and the 2019 Pople Medal of the Asia-Pacific Association of Theoretical and Computational Chemists. Liu has been a member of the Editorial Advisory Board of The Journal of Physical Chemistry since 2017.

19 Surface Hopping Methods for Nonadiabatic Dynamics in Extended Systems

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Due to the ease of implementation and good balance between efficiency and reliability, surface hopping has become one of the most widely used mixed quantum-classical methods for studying general charge and exciton dynamics.¹ In extended systems (e.g., aggregates, polymers, surfaces, interfaces, and solids), however, surface hopping suffers from several severe problems, and thus the relevant applications have been limited in the past years.² Trivial crossings between uncoupled or weakly coupled states have highly peaked nonadiabatic couplings and thus are difficult to deal with in the preferred, adiabatic representation.³ Recently, we systematically classify surface crossings within a time step into four general types and proposed a parameter-free crossing corrected FSSH (CC-FSSH) method to describe the complex nonadiabatic dynamics with a high density of states.⁴ We further showed that a proper choice of subspace can significantly simplify the surface crossings and further increase the performance.⁵ Fast time step convergence and system size independence in systems with thousands of molecular sites have been achieved. In addition, we proposed a branching corrected surface hopping (BCSH) method, which resets the wavefunction coefficients based on the judgement of wave packet reflection.⁶ This approach ensures the self-consistency of using the traditional time-dependent Schrödinger equation for mixed quantum-classical dynamics. As benchmarked in over two hundred distinct scattering models, BCSH has captured the majority of the real decoherence effect, surpassing other existed decoherence correction algorithms. With our recent method developments, complex nonadiabatic dynamics in extended systems could be simulated with improved efficiency and reliability, thus promising for many applications in chemistry, physics, biology, and material sciences.⁷

Keywords: nonadiabatic dynamics; trajectory surface hopping; extended systems; crossing correction; decoherence correction

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110 Infrared Spectroscopy of Neutral Clusters Based on the Tunable Vacuum Ultraviolet Free Electron Laser

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Clusters, consisting of a few to few hundred atoms, exhibit interesting size-dependent properties and bridge the gas and condensed phases.¹⁻³ Currently the studies of clusters focus on the anionic or cationic forms due to ease of size selection and detection, while neutral clusters have presented major experimental challenges as the absence of Coulomb charge makes it difficult for size selection and detection. Dalian Coherent Light Source (DCLS) delivers vacuum ultraviolet free electron laser (VUV-FEL) with a continuously tunable wavelength region between 50 and 150 nm and high pulse energy.⁴ Inasmuch as clusters with different sizes have different ionization energies, the tunable VUV-FEL light paves the way for selectively ionizing a given neutral cluster free of confinement, thus facilitating realization of size selectivity. Here, we report the size-specific infrared spectra of neat neutral water clusters, $(\text{H}_2\text{O})_n$ ($n = 2-6$), based on the tunable VUV-FEL near-threshold single-photon ionization, which lend profound insight to the elucidation of structural evolution in neutral water clusters and provide excellent benchmarks for theoretical study of accurate hydrogen bonding structures of these important clusters.⁵

Keywords: Neutral clusters; infrared spectroscopy; vacuum ultraviolet free electron laser; structure; dynamics

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I11

全息相控阵声镊联姻气液界面质谱

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无论是环境中占地球表面70%的海洋表面和云彩表面, 还是人体中肺部、眼睛和各种粘膜的表面, 均为气液界面。因此气液界面化学的研究对理解气候和污染的生成以及生命体内的关键生化过程都极为重要。然而, 气液界面仅有数十到数百纳米厚, 因此在技术上如何仅采样此极薄的界面层而不受到体相的干扰成为了十分关键的科学和技术问题。针对上述问题, 我们实验室通过自主研发的场致液滴电离-质谱技术, 结合羟基自由基对气液界面分子膜的氧化化学, 攻克了上述技术难关, 系统阐述了界面膜物理行为对其化学行为的影响^[1,2]。

此外, 为了构建完美气液界面, 我们近期又开发了一种先进的全息相控阵声镊技术, 并将其与场致液滴电离-质谱技术相结合, 实现了无容器、悬浮液滴的气液界面研究, 并借此系统阐释了一种光敏抗癌药物的微观作用机理^[3]。

关键词: 质谱; 声镊; 气液界面; 羟基自由基

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复杂体系分子振动能量弛豫问题是理解凝聚相化学动力学的核心。振动模式的能量转移速率决定化学反应途径^[1]。本报告拟介绍我们最近利用振动态选择激发-飞秒时间分辨和频光谱探测技术研究生物膜界面蛋白质振动能量弛豫研究方面的进展。通过选择激发蛋白质酰胺键 N-H 和 C=O 基团, 旨在回答界面蛋白质酰胺键振动弛豫多快, 振动能量如何从 N-H 转移到 C=O, 以及如何从酰胺键转移到周围水溶液环境等问题。通过选择激发 N-H 基团, 然后探测其瞬态结构变化的结果表明 α -螺旋和 β 折叠结构中的 NH 弛豫时间分别是 1.7 和 0.9 皮秒。通过激发 N-H 基团, 探测酰胺键 C=O 瞬态结构变化, 我们的研究表明 N-H 到 C=O 的振动能量传递存在两种途径: 一种是直接的 NH-CO 耦合作用($\sigma_{\text{NH-CO}}$); 另一种是 N-H 先弛豫到某中间态(记为 X 态), 然后 X 态与 C=O 发生耦合作用($\sigma_{\text{X-CO}}$)。系统研究表明 C=O...H-N 的氢键强弱决定 N-H 与 C=O 间两种耦合途径($\sigma_{\text{X-CO}}/\sigma_{\text{NH-CO}}$)的比例。氢键越强, $\sigma_{\text{X-CO}}$ 耦合的比例越高^[2]。通过选择激发酰胺键 C=O 基团, 然后探测其瞬态结构变化, 我们成功测出 H₂O 环境下蛋白质酰胺键 C=O 振动弛豫时间。与 D₂O 情形不同, 暴露于 H₂O 环境的蛋白质残基数量越多, C=O 振动弛豫时间越快(图 1a)。该结果揭示了界面蛋白质与 H₂O 分子弯曲振动在能量上的耦合作用(图 1b), H₂O 分子不仅作为“热库”加快分子内振动弛豫, 而且通过直接的振动共振能量转移通道为蛋白质与溶剂间的能量转移提供“捷径”(图 1c)^[3]。

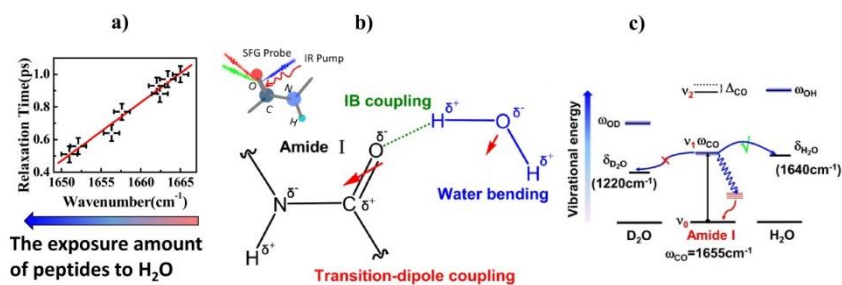


图1、 a) H₂O环境下蛋白质酰胺键C=O振动弛豫时间; b) 酰胺键与水分子耦合作用; c) 酰胺键C=O振动弛豫途径示意图。

Fig.1 a) The vibrational relaxation time of amide I mode against the amide I frequency; b) Interaction between amide carbonyl and water through hydrogen bonding (HB) and transition- dipole coupling; c) Energy-level depiction of the vibrational relaxation of the amide I mode to the water bending mode.

关键词: 界面蛋白质; 酰胺键; 共振能量转移; 飞秒时间分辨和频光谱

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I13 基于单分子光谱的光物理机制研究与超灵敏传感

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单分子光谱技术不仅提供了在分子层面上深入理解化学反应动力学过程与物理机制的可能, 也在可以研究中提供空间分辨的能力。本报告中将介绍我们利用该技术的空间分辨优势深入研究了有机无机杂化钙钛矿材料中光物理机制及淬灭缺陷的本质并利用单分子荧光对扰动的灵敏性实现了室温下微弱振动信号的检测。钙钛矿材料是近几年最热门的材料光伏和光电之一, 其光电转换效率记录不断被刷新。但是由于该材料制备过程的随机性造成材料的差异性较大, 使得对其基础的光物理机制理解还远远不够。因此我们利用单分子光谱技术并结合理论计算, 对于钙钛矿晶体中各种光物理机制特别是淬灭缺陷的本质进行了详细研究, 提出了几种最可能的缺陷的化学本质[1 - 3]。另一方面, 金属纳米颗粒表面等离子体对分子荧光的具有显著的增强效应, 增强因子对分子到纳米颗粒的距离非常敏感, 因此, 通过监测单分子荧光的强度信息, 可以检测分子与纳米颗粒的距离变化, 从而获取环境中造成该距离变化的振动信号, 实现灵敏的振动检测[4]。

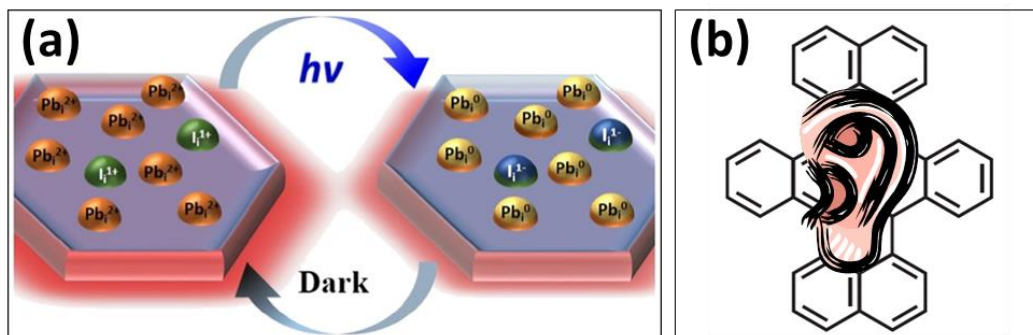


Fig. 1 (a) photo-induced switch between valence states causing PL variation in MAPbI₃. (b) A single molecule can work as an ultra-sensitive vibration detector

关键词: 单分子光谱; 钙钛矿; 缺陷; 振动检测

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I14 Recent Advances in Gas-Surface Reaction Dynamics: High Dimensional Potential Energy Surfaces and Quantum Dynamical Methods

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Gas-surface reactions play an important role in many heterogeneous catalysis processes such as methane steam reformation and water-gas shift reactions. An in-depth understanding of these dynamical processes is of great importance and requires a dynamical model. Due to the large number of degrees of freedom, it is indeed very challenging to model gas-surface reaction dynamics from first principles. Recently, we have developed high-dimensional potential energy surfaces (PESs) including surface atoms for describing the molecule-surface energy exchange, taking advantage of the Behler-Parrinello (BP) type of atomistic neural network (AtNN) method.¹ This approach allows us to perform much more efficient molecular dynamics simulations than on-the-fly ab-initio molecular dynamics (AIMD).² I will show state-to-state scattering results of NO from Au(111), using an AtNN PES. We emphasize the use of an accurate adiabatic PES in describing the vibrational energy relaxation of this system. To further improve the efficiency of the PES, we propose a novel embedded atom neural network (EANN) representation, physically inspired from the well-known embedded atom method.³ Our new implementation is much faster than the BP type of AtNN framework with the same level of accuracy. If there is sufficient time, I will also briefly show preliminary results of using the ring polymer molecular dynamics (RPMD) approach to calculate the initial sticking probabilities of molecules on surfaces. This RPMD method captures quantum tunneling and is immune to the zero point energy leakage, yielding results in excellent agreement with those obtained exact quantum wavepacket method.

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I15 非线性光学研究界面超分子手性形成和传递的分子机理

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表面是构筑手性超分子理想场所, 超分子手性是分子通过非共价键弱相互作用形成的与其镜像不能重合的结构所产生, 在化学、生物学和材料科学研究中具有重要意义。超分子手性研究中一个重要问题是超分子手性是如何产生、传递及分子手性如何影响超分子手性[1]。二阶非线性光学技术, 包括二次谐波(SHG)及和频光谱(SFG)已被证明不仅具有界面选择性和敏感性, 而且是手性敏感的技术。本研究中, 我们将主要讲述本课题组近年来在界面超分子手性自组装分子机理方面部分工作: (1) 利用手性二次谐波和手性和频光谱研究具有同分异构体的席夫碱衍生物两亲分子气液界面上自组装形成手性聚集结构机理。这两种分子虽然具有相同的手性中心, 但组装形成的超分子结构具有截然相反的手性方向, 此外, 还研究了在不同外场和不同金属离子配位下所形成的超分子手性结构的分子机理, 提出了一种超分子手性界面形成的分子机制, 解释了界面超分子手性形成与分子结构的关系。(2) 利用手性二次谐波和频光谱研究了谷氨酸衍生物界面超分子手性传递的分子机理, 本研究发现谷氨酸衍生物的中酰胺键的数目对于超分子自组装手性具有重要作用, 该研究对于界面超分子构筑单元的选择和合成具有指导意义。

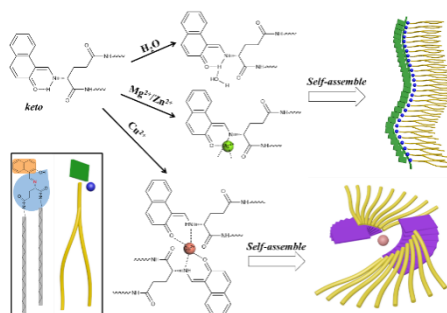


Fig. 1 The proposed model of self-assembly mechanism and chiral formation of LGJ at air/water interface with pure water, Mg^{2+} , Zn^{2+} , and Cu^{2+} ions in the subphases

关键词: 超分子手性; 界面; 自组装; 手性二次谐波; 手性和频光谱

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116 Ultrafast Relaxation Dynamics of Photoexcited Fluorophenols

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As one of the most important chemical and biological building blocks, the relaxation dynamics of photoexcited phenol have received a lot of attention. Previous research has confirmed experimentally that photodissociation of phenol is correlated with the H atom on O-H bond tunneling through the barrier under S_1/S_2 conical intersection [1-3]. In this work, using femtosecond pump-probe technique, time of flight mass spectroscopy, and ion velocity map imaging, we have investigated the photodissociation dynamics of the derivatives of phenol at a series of wavelengths. With the help of quantum chemical calculations, we try to understand the role of tunneling which plays in their H-elimination dynamics. As for m-fluorophenol, following excitation to S_1 state below the S_1/S_2 CI, we have observed H atoms with high kinetic energy which we assign to yielding from tunneling beneath the S_1/S_2 CI, followed by coupling onto the dissociative S_2 state. This tunneling mechanism is confirmed by studies on the selectively deuterated species, m-fluorophenol-d1. Meanwhile, our quantum chemical calculations have also provided relevant evidence for the consequence. However, the photodissociation dynamics is quite different for photoexcited o-fluorophenol, an extra photodissociation channel is observed, which is absent for the relaxation of photoexcited m-fluorophenol. Our results highlight the effect that the presence of additional functional group F, and more specifically the precise location of the functional group, can have on the dissociation dynamics of phenols. Furthermore, by introducing a third femtosecond infrared laser on the photoexcited molecules, we are able to modify the H-elimination process, observing the change of the tunneling time and also the different H-elimination channels.

Keywords: pump-probe; ultrafast; photodissociation; velocity map imaging

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117 Strong and Selective Isotope Effect in the Vacuum Ultraviolet Photodissociation Branching Ratios of Carbon Monoxide

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Rare isotope (¹³C, ¹⁷O and ¹⁸O) substitutions can substantially change absorption line positions, oscillator strengths and photodissociation rates of carbon monoxide (CO) in the vacuum ultraviolet (VUV) region, which has been well accounted for in recent photochemical models for understanding the large isotopic fractionation effects that are apparent in carbon and oxygen in the solar system and molecular clouds [1, 2]. Here, we demonstrate a strong isotope effect associated with the VUV photodissociation of CO by comparing the branching ratios of ¹²C¹⁶O and ¹³C¹⁶O. The measurements show that the quantum yields of electronically excited C atoms in the photodissociation of ¹³C¹⁶O are dramatically different from those of ¹²C¹⁶O, revealing strong isotope effect. This isotope effect strongly depends on specific quantum states of CO being excited, which implies that such effect must be considered in the photochemical models on a state by state basis [3].

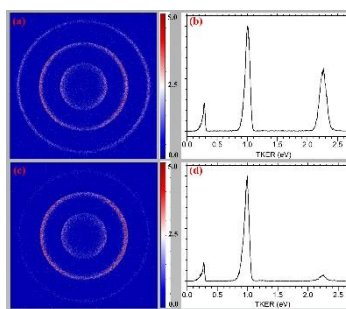


Fig. 1 The raw time-slice velocity-mapped ion images and the corresponding total kinetic energy release (TKER) spectra for VUV photodissociation of ¹²C¹⁶O ((a) and (b)) and ¹³C¹⁶O ((c) and (d)) in the ¹Π (v'=2) state at 107685.8 cm⁻¹. The three peaks in the TKER spectra are for the three dissociation channels C(³P) + O(¹D), C(¹D) + O(³P) and C(³P) + O(³P) with increasing TKER.

Keywords: Isotope effect; photodissociation; branching ratio; vacuum ultraviolet; carbon monoxide

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118 Probing the Stability and Reactivity of Metal Clusters

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The study of stable/unstable clusters provides information bridging the gap between atoms and macroscopic bulk materials, among which the insights of the reactivity of metal clusters facilitate a better understanding of the fundamentals in metal surface chemistry by revealing the interaction mechanism between metals and adsorbent.^[1] Well-resolved Ag_n^+ clusters are produced by a self-designed magnetron sputtering source (MagS) as well as a home-made LaVa source. Utilizing customized reflection time-of-flight mass spectrometer (Re-TOFMS)^[2] and Selected Ion Flow Tube Reactor in tandem with Triple Quadrupole Mass Spectrometer (SIFT-TQMS), we systematically studied the ion–molecule reactions between metal clusters and polar/nonpolar molecules. It is found that a few stable metal clusters survive the oxygen etching reactions; however, certain ionic clusters readily react with oxygen leading to the production of both etched building blocks and oxygen-rich species profiting from the ion–molecule attraction and hence increased collisional cross section. The finding of synchronous channels of both etching and growth of certain metal clusters clarifies the reactivity of metal clusters with oxygen, interprets the readily formed metal-oxide and enriches the understanding of the industrial chemistry of metals.^[3] Besides, determined by the weak noncovalent interactions, the gas phase reaction of certain metal clusters with hydrocarbons (e.g., acetylene) offers different viewpoints of the metal cluster reactivity. For example, on the reactions of silver cluster cations with acetylene under sufficient collisional conditions, only $\text{Ag}_7^+[\text{C}_2\text{H}_2]$ was observed as a product with reasonable intensity. The joint experimental and theoretical study reveals that the Ag_n^+ clusters do not form strong Ag-C bonds with C_2H_2 , and $\text{Ag}_7^+[\text{C}_2\text{H}_2]$ bears larger binding energy than the other $\text{Ag}_n^+[\text{C}_2\text{H}_2]$ although within similar cluster- π interactions. The metal-involved noncovalent interaction bonds in $\text{Ag}_7^+[\text{C}_2\text{H}_2]$ is fully demonstrated via the topological analysis and NBO analysis, together with both thermodynamics and kinetics discussion.^[4] More details of the recent advances in probing the stability and reactivity of metal clusters will be given by the oral presentation.

Keywords: metal reactivity; ion–molecule interaction; cluster– π interaction; mass spectra; gas phase

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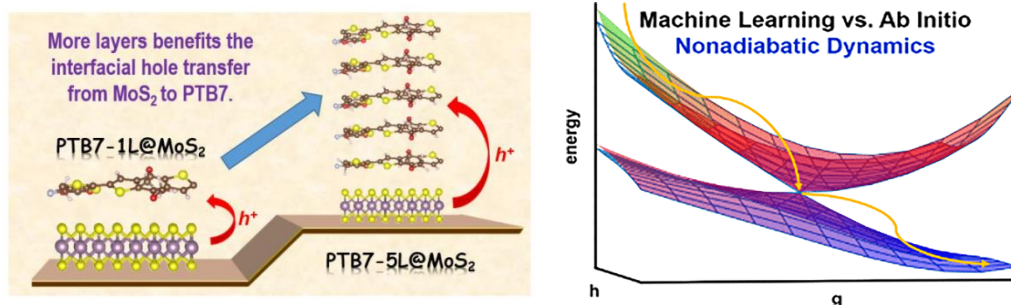
从头算非绝热动力学方法及其应用

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化学、生物、材料、大气等研究领域都涉及极其复杂的光物理和光化学。计算模拟，特别是从头算模拟，在理解实验现象背后的微观物理机制、预测实验、理性设计等方面起着十分重要的角色。同时，我们需要进一步发展适合不同复杂体系的激发态电子结构和非绝热动力学方法，提高精度和效率。在本报告中，我主要汇报课题组在过去几年间在非绝热动力学方法及其在化学、生物及材料体系方面的一些工作。首先，简单介绍课题组发展的能同时处理内转换和系间窜跃的非绝热动力学方法；为了提高模拟效率，我们进一步发展了非绝热和旋-轨耦合的算法，并用于模拟量子点和有机金属体系的激发态弛豫及界面间的载流子迁移动力学。最后，介绍一下课题组，在利用机器学习和低标度的激发态电子结构方法进行激发态计算和非绝热动力学模拟方面的一些探索工作。



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120 Photodynamics of Criegee Intermediates: The Effects of Methyl and Vinyl Substitution

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The photochemistry of Criegee intermediates (CIs) plays a significant role in atmospheric chemistry but is relatively less known compared with their thermal reactions. Using multireference CASPT2 electronic structure calculations and CASSCF trajectory surface-hopping (TSH) molecular dynamics, we have revealed the unimolecular photochemical reactions of simplest CI (CH_2OO , sCI)^[1] as well as the methyl and vinyl substituted CIs (CRHCOO , $\text{R}=-\text{CH}_3, -\text{CH}=\text{CH}_2$), etc. In addition to the known photodissociation channel^[2], a dark-state involved $A^1A \rightarrow X^1A$ photoisomerization channel to a cyclic dioxirane has been found. The molecule on A^1A state is driven by the out-of-plane motion to reach a perpendicular A/X^1A minimal-energy crossing point (MECI), then nonradiatively decays to the ground state. The dynamics of these processes, including the excited-state lifetime, hopping probabilities and product quantum yields have been revealed by the TSH simulations. For both the unsubstituted and substituted CIs, the A/X^1A -CI acts as a funnel for the syn-anti interconversion and ring-closure channels, but the quantum yields for different channels are significantly affected by the substituents. These findings expected to broaden the reactivity profile and deepen the understanding of the photochemistry of Criegee intermediates.

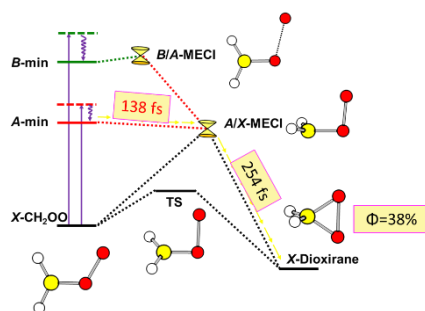


Fig. 1 A dark-state-involved $A^1A \rightarrow X^1A$ photoisomerization channel of CH_2OO leading to a cyclic dioxirane.

Keywords: Criegee Intermediate; Molecular Dynamics; Photodynamics; Multireference ab initio Method

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钙钛矿材料激发态动力学

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含卤素的钙钛矿太阳能电池具有较高的光电转换效率，近年来受到广泛关注。材料的微观结构如晶界、掺杂、空气湿度、氧气、有机阳离子重排和无机框架扭曲等因素强烈影响非辐射电荷和能量损失以及器件性能。通过含时密度泛函理论结合非绝热动力学模拟，我们研究了多种实际因素对钙钛矿材料光生电子转移[1]和电子-空穴复合[2-13]动力学的影响，获得了该复杂体系详细的电子-振动动力学信息，厘清了大量实验和理论上存在争议的科学问题，为提高钙钛矿材料光捕获能力和降低能量损失提供了有价值的理论指导。

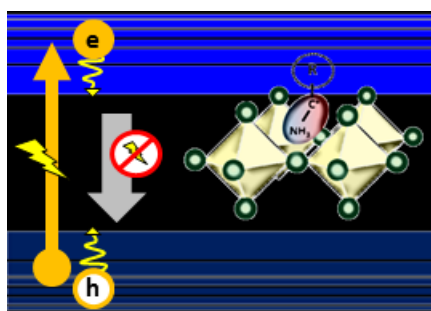


Fig.1 钙钛矿电池的光诱导载流子动力学

关键词：钙钛矿，缺陷，电子转移，非辐射电子-空穴复合，非绝热动力学，含时密度泛函理论

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I22 Probing Geometric Phase Effect in $\text{H}+\text{HD}\rightarrow\text{H}_2+\text{D}$ via Energy Dependent state Specific DCS Oscillations and Rotational State Distribution

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Geometric phase (GP) effect in chemical reaction has been an interesting topic in reaction dynamics for a long time^{1,2}. Recently, GP effect been observed for the first time in a chemical reaction using the high-resolution velocity mapping imaging - crossed beams method.³ Geometric phase effect was clearly detected in the oscillatory angular distribution of the H_2 product from the $\text{H}+\text{HD}\rightarrow\text{H}_2+\text{D}$ reaction. Recently we tried to probe the GP effect in $\text{H}+\text{HD}\rightarrow\text{H}_2+\text{D}$ by measuring collision energy dependent differential cross section (DCS) for a specific H_2 product state. Oscillatory structure of energy dependent DCS of $\text{H}+\text{HD}(v=0, j=0)\rightarrow\text{H}_2(v'=2, j'=3)+\text{D}$ in the backward-scattering direction at collision energy between 1.94 and 2.21 eV. We also prepared $\text{HD}(v=1, j=2)$ with selected alignment, and measured the ro-vibrational state distribution of H_2 product from $\text{H} + \text{HD}(v=1, j=2) \rightarrow\text{H}_2+\text{D}$ at a fixed collision energy of 2.07 eV in the forward-scattering direction. Both experimental results are in excellent agreement with adiabatic quantum dynamical calculations with inclusion of GP, demonstrating the existence of GP effects at collision energy far below the conical intersection of this benchmark reaction.

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真空紫外单光子电离质谱/光谱技术及其应用

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真空紫外单光子电离是一种“软电离”技术。应用真空紫外单光子电离和飞行时间质谱技术, 以可调谐的红外光作为激发光源。在本报告中, 我们将报道本课题组在气相中氢键团簇的红外光谱和分子结构的最新研究结果。最近, 应用自主搭建的质量选择的串级质谱设备, 课题组开展了对不同质量大小的团簇离子的红外光谱的探测, 以118 nm真空紫外激光作为电离光源, 在超声射流中制备出分子团簇, 应用质量分辨的IR-VUV光谱方法和质量选择的红外多光子解离光谱 (IR-MPD) 方法对几种典型氢键团簇体系的中性和离子体系进行了探测研究。结合高水平DFT理论计算, 模拟出体系的红外光谱, 并与实验探测所获得的红外光谱进行比对, 对团簇离子可能存在的分子结构进行确认, 并对团簇内单体间发生的分子间相互作用动力学过程进行了深入探讨。

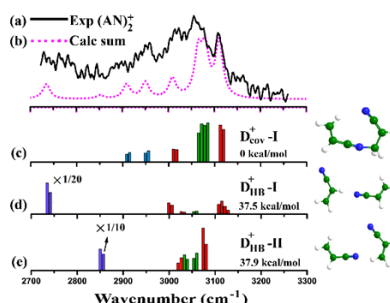


Fig. 1 (a) Observed and (c-d) calculated IR spectra of cationic AN dimer.

关键词: 氢键团簇; 单光子电离; 红外光谱; 串级质谱; 团簇结构

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124 Solvent Effect on Triplet-triplet Annihilation Upconversion of Perylene with Bodipy-fullerene Photosensitizers

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Solvent effect usually plays an important role in triplet-triplet annihilation (TTA) upconversion process [1,2]. Recently, we have synthesized a series of new metal-free photosensitizers of bodipy-fullerene. All these dyads have as long triplet lifetime as microseconds. Using these photosensitizers, the kinetics of TTA upconversion fluorescence emission of perylene were investigated in several solvents, e.g., 1,4-dioxane, toluene, chlorobenzene, dichlorobenzene, and tetrahydrofuran. The femtosecond and nanosecond transient absorption spectroscopy was performed to measure the intra- and inter-molecular energy transfer rates. The TTA upconversion quantum yields were determined then. With the aid of cyclic voltammetry and ab initio calculations, the physical and chemical mechanisms of the overall processes were proposed. Of special interest was that a nonsignificant dependence on solvents was found in the system, except for fluorescence emission of perylene itself.

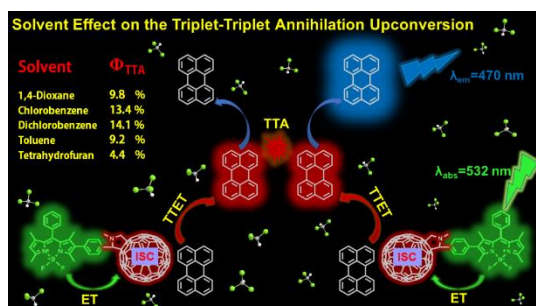


Figure 1. Solvent effect on TTA upconversion of perylene with C60-Bodipy as photosensitizers.

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125 利用离子切片速度成像对金属原子氧化反应的动力学研究

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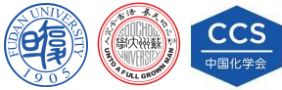
我们利用交叉分子束和时间切片离子速度成像技术对金属原子氧化反应中的电子转移动力学开展了实验研究。其中在Al($^2P_{1/2,3/2}$)原子的氧化反应动力学研究中, 对AlO进行了(1+1)选态共振电离探测。AlO的转动常数较小, 被激发到的最高转动态AlO产物测到的速度几乎为零, 表明可利用能量几乎全部分配到产物的转动能上。根据角动量守恒, 测得AlO的最大转动态N=52对应的反应碰撞参数为 $2.5 \pm 0.2 \text{ \AA}$, 与理论计算得到的电子转移距离一致, 并与渔叉机理模型预测的电子转移距离一致, 从而首次在实验上真正验证了这一理论模型, 即电子转移距离与反应物的电离势和电子亲和能之差有关。产物角分布随着产物角动量的增加由前后向分布趋向于各向同性, 表明随着转动量子数的增加, 产物几乎忘记初始速度方向。前后向产物散射分布表明有寿命较长的中间产物生成。前向比后向较强表明大部分中间产物的寿命低于一个转动周期。

此外, 我们对过渡金属原子Y和O₂/SO₂/NO的氧化反应动力学进行了研究。基态Y($a^2D_{3/2}$)与O₂/SO₂/NO反应焓变 ΔH 由小到大分别为-52.8 kcal/mol, -33.9 kcal/mol, -13.7 kcal/mol。放热多少对产物YO的内能态分布产生主要影响。Y和O₂/SO₂反应产生YO电子激发态, 包括A² $\Delta_{3/2,5/2}$ (41.5, 42.5 kcal/mol)和A² $\Pi_{3/2,5/2}$ (46.6, 47.9 kcal/mol)。电子激发态产物YO的角分布显示出前后向散射较强的分布, 表明有寿命较长的中间产物生成, 前向比后向强, 表明大部分中间产物的寿命低于一个转动周期。Y和O₂/NO反应产生可分辨的振动激发态的YO($X^2\Sigma^+$), 其前后向散射角分布表明有寿命低于一个转动周期的中间产物生成。电子转移形成的离子对络合物可用于解释过渡金属原子氧化反应动力学过程。

关键词: 金属原子反应动力学; 速度成像; 交叉分子束; 电子转移

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张未卿

先进光源的发展在前沿科学研究中发挥的作用越来越重要。近几十年来，自由电子激光技术的突破为科学家们提供了探索未知世界、发现新科学规律、实现技术变革的重要工具。自由电子激光技术的发展推动物质科学的实验研究由宏观体系深入到单个原子和分子尺度体系、从静态过程到超快的动态过程、从理想实验环境下的研究逐步转向接近真实反应条件下的研究。具有高亮度、超快特性的极紫外自由电子激光可以高效地激发原子分子的外层电子并电离分子自由基，将实现科学家在原子分子层次，同时在超快时间尺度上研究重要的物理、化学、生物过程的梦想。大连相干光源是由国家自然科学基金委资助、由中科院大连化学物理研究所和上海应用物理研究所共同承担的重大科学仪器研制项目，是一种以相对论高品质电子束作为工作介质，在周期磁场中以受激发射方式放大电磁辐射的新型强相干激光光源。光源的单个皮秒激光脉冲能量超过 100 μ J，重复频率 50Hz，波长在整个极紫外区域（50-150nm）完全连续可调，具有完全的相干性。2017 年 1 月，大连光源首次出光，脉冲能量达到 210 μ J。建成的大连相干光源是我国第一台大型自由电子激光科学研究用户装置、当今世界上唯一运行在极紫外波段的自由电子激光装置。目前，光源已经给用户 provide 高亮度的极紫外激光，并有初步的实验结果。本报告将主要介绍光源性能、应用及未来发展计划。

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低能量离子-分子反应动力学研究进展

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低能量离子与分子的碰撞反应主要包括电荷交换及其后续的化学反应, 是星际空间、大气和溶液中的重要物理化学过程。目前, 相比于中性原子(自由基)-分子碰撞反应研究, 离子-分子反应动力学研究还很薄弱。最近, 我们研究组研制了时空约束脉冲化低能量离子束源, 并结合离子速度成像技术, 组建了一台低能量离子-分子的交叉束反应装置。该装置的探测器由最初的荧光屏-CCD相机组合更换为延迟线阳极(如图所示), 提高了探测效率并且可以获得产物离子的三位Newton球速度影像。利用该装置, 我们初步完成了低能量 Ar^+ 离子与 NO 、 N_2 、 CO_2 、 O_2 等分子的反应动力学研究。本报告中将对上述研究进展进行了总结, 并对实验技术的改进和未来研究内容进行展望。

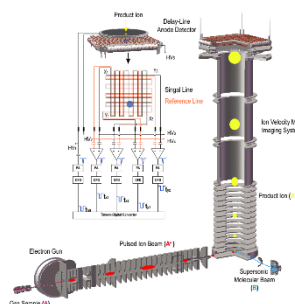


Fig. 1 Schematic of our experimental apparatus.

关键词: 离子-分子反应; 电荷交换; 星际化学; 大气化学



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钙钛矿光伏器件中的载流子动力学研究

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钙钛矿光伏器件是近年来发展迅速的研究领域, 其内在光电转换机制特别是光生载流子的动力学行为对深入了解该新型电池具有重要意义。我们研究了从薄膜到光伏器件多个维度的本征属性及载流子复合动力学。利用变温荧光/吸收光谱和时间分辨荧光等光谱手段研究本征钙钛矿带隙内的缺陷态分布情况, 以及带边/缺陷态的辐射复合过程, 获得了辐射/非辐射复合临界能、缺陷态捕获电子的脱附活化能和特征温度等参量。在介孔结构器件中发现了两相式的电荷累积与载流子复合机制, 提出了Multiple-Trapping载流子复合模型, 同时揭示了填充因子与缺陷态性质的内在联系。利用时间分辨光动力学分析比较了不同器件结构对电荷累积、载流子传输和复合性质的影响, 并讨论了钙钛矿器件中滞后现象可能的结构因素。在开路、短路和工作条件下考察了瞬态光电转换动力学, 揭示功率输出和载流子复合和传输动力学过程的相关性。

关键词: 钙钛矿太阳能电池; 瞬态吸收光谱; 瞬态光动力学; 缺陷态

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O2 Rotational Pursuits on Internal Dynamics in Non-Covalent Bonded Molecular Complexes

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Rotational spectroscopy is a uniquely precise tool for the determination of molecular structure, conformational behaviors, non-covalent interaction and internal dynamics in gas phase. The internal dynamics raised from the large amplitude motions (LAMs) is one of the interesting features in rotational spectra of non-covalent bonded molecular complexes, which are characterized with tunneling splittings of rotational transitions. The width of these splittings are contributable to the corresponding rotational states, the orientations of the internal rotors in molecules, and the barriers to LAMs. Thanks to its intrinsic high resolution, the experimental data of the barrier height to the LAMs are also benchmark for theoretical calculations.

In this contribution, several rotational studies on non-covalent bonded molecular complexes will be taken as examples to showcase the capability of pulsed-jet Fourier transform microwave spectroscopy combined with theoretical calculations in describing the internal dynamics, such as the pathway and the barrier height to internal rotation of water^[1] and the methyl groups,^[2] or the proton transfer in hydrogen bond.^[3]

Keywords: Internal Dynamics; Molecular Complexes; Rotational Spectrum; Barrier height; Fourier transform microwave spectroscopy

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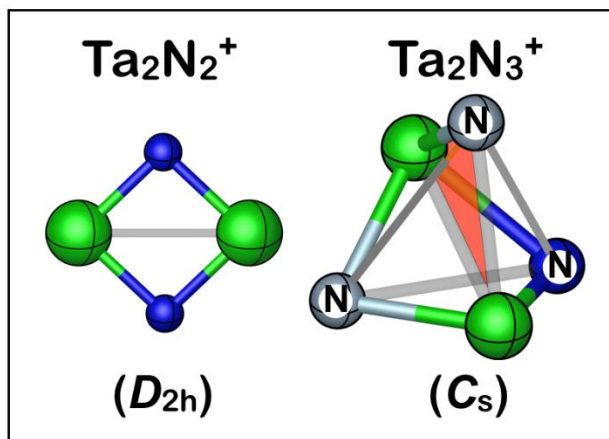
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氮气是空气的最主要成分, 取之不尽用之不竭。但是氮气分子是最稳定的分子之一, 温和条件下氮气的活化与转化是当今催化化学的重要挑战之一。我们发挥理论计算的前瞻性, 设计了一种“由空气制面包”的方法, 即使用原子簇 Ta_2^+ 作为调控氮气和氢气的催化剂在室温条件下合成氨。此偶联模拟了工业上极其重要的由 N_2 和 H_2 合成氨的“Haber-Bosch”过程^[1,2,3]; 确定了正向过程(即 N_2 活化)和逆向过程(即原子簇调控 NH_3 分解)的关键步骤。 $Ta_2N_2^+$ 是正、逆向路径的必经中间体(如图, $Ta_2N_2^+$)。根据化学微观过程可逆性, 正逆反应的结合完美的构成了室温下合成氨的可行途径^[4]。

催化剂通过开启能量有利的途径加速化学反应。尽管催化过程普遍存在, 但实际的催化活性物种常常难以捕捉: 催化剂和底物之间的相互作用通常很快, 短寿的活性中间体难以鉴定。延续 Ta_2^+ 调控氮气和氢气合成氨的工作, 我们尝试理性修饰 Ta_2^+ , 将两金属原子间桥连一个N原子, 实验上合成得到 Ta_2N^+ 。非常令人兴奋的是, 这个微小的“分子机器”可在室温下切断非常强的 N_2 叁键并进行重新组装。反应经由具有两个相同化学环境的N原子的中间体是反应发生N原子交换、“催化剂” Ta_2N^+ 再生的前提(如图, $Ta_2N_3^+$)。对 $Ta_2^+/Ta_2N^+/Ta_2N_3^+$ 三个体系中金属前线轨道能量分析揭示了 N_2 活化的关键因素: 金属 π -反馈轨道能量越高, 反应活化能垒越低^[5]。

Fig. 1 Global minima of $Ta_2N_2^+$ and $Ta_2N_3^+$.

关键词: 气相催化; 氮气活化; 活性位点; 合成氨; 量化计算

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O4 磷脂膜表面分子行为的二次谐波与荧光探测研究

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理解磷脂膜表面药物与染料分子的结构与动力学行为在生物染色、药物负载和药物作用机理研究中都具有重要的意义。二阶非线性光学技术(二次谐波与和频振动光谱)因其界面选择性与单分子层灵敏探测能力[1], 在载药囊泡、细菌、细胞膜表面分子结构与动力学行为研究中都做出了突出的贡献。近期, 我们使用二次谐波这种界面选择性的技术与荧光光谱这种理论上不具有界面选择性的技术, 对一些染料和药物分子在囊泡表面的吸附、聚集、嵌入和跨膜传输等动力学行为进行了深入的研究[2, 3]。利用分子在不同化学环境中荧光效率显著变化的特性, 我们将荧光光谱也作为一种具有界面选择性的光谱学方法, 并利用其得到了对药物与染料分子界面动力学行为的细致认识。我们通过此研究获得了离子强度对囊泡表面分子吸附和传输行为的显著调控作用, 同时对具有不同结构、不同电荷的分子在不同磷脂膜上的结构、荧光效率以及它们对磷脂膜传输性能的影响进行深入分析。

关键词: 囊泡, 磷脂膜, 二次谐波, 荧光, 界面

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O5 用慢电子速度成像方法精密测量过渡族和镧系原子电子亲和势

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电子亲和势是反映原子分子和电子结合能力的一个基本参数, 对化学反应、等离子物理、大气物理化学、天体物理等多个领域都很重要。目前, 很多过渡族和绝大多数镧系元素的电子亲和势还是未知的, 有报道的实验测量值误差也较大, 约10 meV。由于 f 电子子壳层和 d 电子子壳层没有填满, 过渡族和镧系元素原子负离子电子结构非常复杂, 无论是理论计算还是实验测量仍然是一个很大的挑战。传统的光电子能谱仪的典型能量分辨率10 meV, 很难分辨其电子结构, 这是大多数过渡族及镧系原子的电子亲和势还没有实验测量值或测量精度不高的根本原因。最近, 我们利用慢电子速度成像方法对过渡族和镧系元素的电子亲和势成功进行了精密测量, 还同时得到了其负离子能级的精细结构劈裂。将质谱、低温离子阱、慢电子速度成像三种方法联用, 可以实现0.5 meV的能量分辨率, 可以很好分辨镧系原子分子的复杂电子结构, 同时很好解决了氢化物同位素干扰问题, 可以把电子亲和势的测量精度提高到好于0.1 meV[1-5]。目前, 利用这个方法我们已经完成了二十多个元素电子亲和势的测量。此外, 利用冷离子阱技术, 我们可以将分子负离子的温度冷却到~10K, 可以大大降低分子负离子的光电子能谱的热展宽。高分辨谱学数据将为发展相应的理论计算方法提供严格的检验, 帮助人们更好地认识过渡族及镧系金属元素的性质。

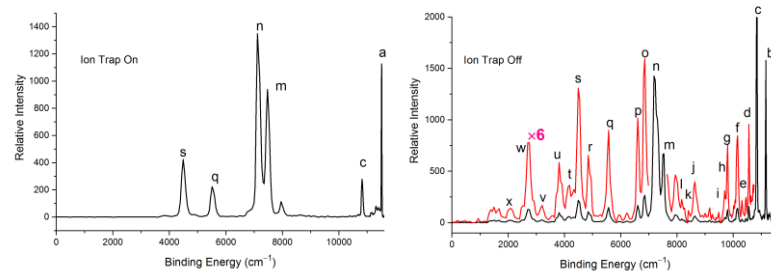


Fig. 1 Photoelectron spectra of La^- at photon energy $h\nu = 11595.57 \text{ cm}^{-1}$ obtained with the trap-on mode (left) and the trap-off mode (right). In the trap-on mode, the ions are trapped for 45 ms, and are then thrown out for further analyzing. In the trap-off mode, the ions directly fly through the ion trap as the trap is turned off. The red curve shows the weak peaks multiplied by a factor of 6 for a clearer view. More excited states were observed in the trap-off mode.

关键词: 过渡族; 镧系; 电子亲和势; 慢电子速度成像; 冷离子阱

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O6 Catalytic CO Oxidation by O₂ Mediated with Neutral Heteronuclear Metal Oxide Clusters

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Study of heteronuclear metal oxide clusters (HMOCs) that are promising models for the active sites on widely used mixed metal oxide catalysts is important to uncover the molecular-level mechanisms in related bulk systems. However, the current reactivity studies of HMOCs are focused on charged clusters with little attention paid on neutral species. Reactivity study of neutral HMOCs is vital to have a comprehensive understanding on heterogeneous catalysis because the active sites on real-life catalysts can be positive, negative, or neutral in nature. It is experimentally challenging to study neutral clusters due to the difficulties of cluster ionization and detection without fragmentation. In our recent works, we presented the advances in the reactivity studies of neutral HMOCs in catalytic CO oxidation. We discovered the reactivity of neutral AuTi₂O₃₋₆ clusters for catalytic CO oxidation. The crucial roles of the mobile AuCO species that can facilitate both processes of CO oxidation and O₂ activation have been emphasized. Furthermore, we discovered that a four coordinated iridium site in neutral IrAl₂O₈ cluster can also catalyze CO oxidation, and the important roles of lattice oxygen that can modify the coordinated environment of the iridium site can then the reactivity of four-coordinated iridium were explored.

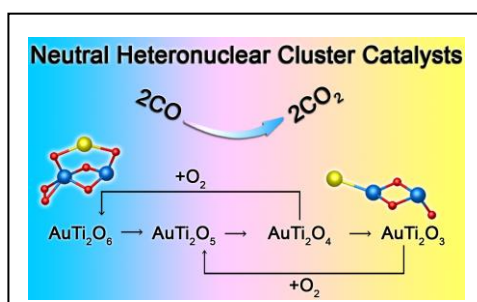


Fig. 1 Neutral Au₁-Doped Cluster Catalysts AuTi₂O₃₋₆ for CO Oxidation by O₂

Keywords: neutral clusters; catalytic CO oxidation; mass spectrometry; DFT calculations

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07 基于时间分辨共振拉曼光谱技术对光化学反应过程中重要短时中间体的结构识别

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光诱导反应后体系激发态衰减通道往往较为复杂，各种低能激发态、短时中间体常常共存，若它们的电子吸收或荧光峰相近或重叠、寿命相似，会使其精准指认造成困难。目前对于相关光化学反应过程中激发态与短时中间体结构的准确指认仍是亟待解决的难题。而对光化学反应过程中重要短时中间体物种的结构准确解析与识别是研究、阐明其反应机理的必要途径。利用时间分辨共振拉曼光谱捕捉短时物种的特征指纹光谱，结合量子化学理论计算确定物种结构，能对洞悉激发态的衰减通道和重要中间体形成机理提供独特的结构信息。本报告将以光解芳香叠氮化合物产生氮宾离子，和其与DNA鸟嘌呤反应生成C-8加合物体系，以及硝基多环芳烃三重激发态 (T_1) 的氢转移反应体系为例，介绍基于时间分辨共振拉曼光谱技术在识别短时中间体结构中的重要应用。

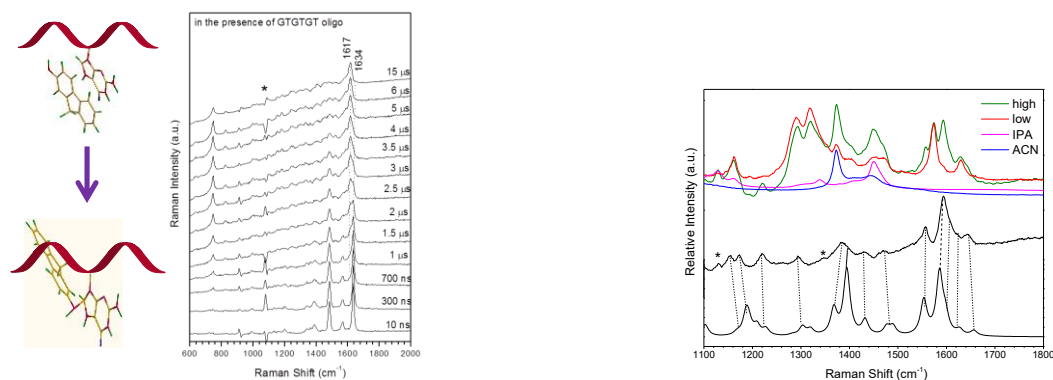


Fig. 1 (left) Time-resolved resonance Raman spectra after laser photolysis of 2-fluorenyl azide in the presence of d-GTGTGT oligo in buffered aqueous solution, and (right) comparison of single pulse resonance Raman spectrum of 4-nitro-1-naphthol in alcoholic solution to the DFT calculation predicted normal Raman spectrum for candidate structure.

关键词： 时间分辨；共振拉曼；短时中间体

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08 甲烷等离子体辅助燃烧中O₂(¹Δg)的动力学效应张凤^{1,*}, 黄灿¹, 谢斌斌², 申林³¹中国科学技术大学国家同步辐射实验室, 安徽省合肥市合作化南路 42 号, 230026²浙江师范大学高等研究院, 杭州市萧山高教园区耕文路 1108 号, 311231³北京师范大学化学学院, 北京市新街口外大街 19 号, 100875

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氧气分子与燃料自由基反应的化学动力学过程, 尤其是链分支、链传播和链终止反应的竞争关系, 是常规燃料低温着火的关键。在等离子体辅助燃烧背景下, 部分氧气分子被激发到电子激发态(¹Δg)。处于电子激发态的氧气分子与燃料自由基可能在更低温度下触发链式反应, 从而对着火动力学包括着火和火焰传播等产生不可忽视的影响。然而, 无论是从实验还是理论角度针对激发态氧气的反应动力学展开研究都面临极大挑战。本工作选择甲烷作为燃料分子, 通过理论计算手段包括量子化学方法、RRKM/主方程方法和燃烧动力学模拟, 探讨在等离子体辅助燃烧的极端条件下, 激发态氧气分子(¹Δg)参与的化学反应对燃烧动力学的影响。

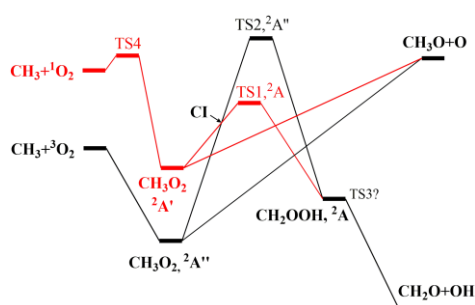


图 1. 甲基与基态和激发态氧气反应势能面示意图

关键词: 等离子体辅助燃烧; 甲烷着火机理; RRKM/主方程方法; 燃烧动力学模拟; 激发态氧气

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O9 Orientation Assignment of LH2 and LH1-RC Complexes from *Thermochromatium tepidum* Reconstituted in PC Liposome and Their Ultrafast Excitation Dynamics Comparison Between in Artificial and in Natural Chromatophores

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The light-absorbing pigments in purple photosynthetic bacteria are organized into two transmembrane pigment-protein complexes, i.e. the peripheral LH2 complexes and the core LH1-RC complexes. In most species, the light energy is initially captured by LH2 and is then transferred via LH1 to the RC. In this study, the artificial chromatophore was constructed by reconstitution of light-harvesting complex 2 (LH2) and core-complex (LH1-RC) from *Thermochromatium tepidum* in egg phosphatidylcholine (PC) liposome. By calcium ion dependent absorption changes, the orientations of protein complexes in liposomes solely were assigned. Ultrafast EET dynamics were studied by fs time-resolved absorption spectroscopy on both the artificial and natural chromatophores at their RC 'open' and 'close' states, respectively. The results indicated that these two membrane systems have similar EET dynamic profiles, and the orientations of LH2 and LH1-RC complexes in artificial chromatophores were opposite to those in natural chromatophores.

Keywords: *Thermochromatium tepidum*; Pigment-protein complex; Reconstitution; Ultrafast excitation energy transfer; dynamics

O10 无机/有机界面三线态能量转移动力学及其光学上转换应用

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近年来,通过无机纳米晶到多环芳烃的三线态能量转移(TET)驱动三线态-三线态湮灭光学上转换(TTA-UC)开始受到研究人员的广泛关注。这一上转换途径具有能量增益大、阈值低等优势,有望解决太阳转换中的低能光子的透过损失。但是,在基础研究层面TET的机理还很不清晰,这是因为传统纳米晶表面的缺陷态使得TET过程过于复杂化。在本工作中,我们采用近期广受关注的钙钛矿纳米晶作为三线态给体进行TET机理研究;这类纳米晶发光效率高(70%),可使缺陷态对界面TET的干扰最小化。采用CsPbBr₃纳米晶-多环芳烃模型体系,通过细致的超快光谱学研究,我们揭示了TET中的若干基本原理:¹(1)TET速率与纳米晶隧穿到表面的波函数平方成正比,表明了波函数交叠在TET中的决定性作用;(2)当多环芳烃的能级结构允许和禁阻纳米晶到其的电荷转移通道情况下,TET分别由实和虚的电荷转移态介导。在这些基本原理的指导下,我们设计出了基于CsPbBr₃纳米晶-多环芳烃体系的高效率的可见到紫外上转换体系。^{2,3}除钙钛矿纳米晶的本子激子态TET以外,我们还采用CuInS₂纳米晶作为模型体系研究了缺陷态激子的TET动力学。发现该体系的自缺陷激子TET转移速率确实较慢,但受益于自缺陷激子的长激发态寿命,能量转移效率仍可大于90%,并可用于高效率的TTA-UC。⁴

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O11 Charge Separation Initiated by Intramolecular Charge-transfer

Excitations in All-polymer OPV Blends

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The performance of organic solar cells has been dramatically improved in the last few years by employing non-fullerene electron acceptors. The charge separation yield at a bulk heterojunction sets the upper efficiency limit of an organic solar cell. Previous studies in polymer/fullerene blends suggest that charge separation is mainly enabled by dissociation of Frenkel excitons absorbed by polymer donors. Here, we show that interfacial charge separation in multiple high performance all-polymer junctions can occur through a charge-transfer-state (polaron pair) derived hole transfer, which is a fundamentally different mechanism compared to the exciton-dominated pathway in the polymer/fullerene blends [1]. By utilizing ultrafast transient absorption measurements, we have clearly identified an ultrafast hole transfer process with a lifetime of about 3 ps mediated by photo-excited charge-transfer states which has a markedly high quantum efficiency of about 97%. Spectroscopic data show that Frenkel excitons act as spectators during the efficient hole transfer process. Further studies using two-dimensional electronic spectroscopy [2] have shown the coherent formation of Frenkel excitons and charge-transfer excited states in sub-100 fs which undergo different dynamical channels at a late stage. Our findings suggest an alternative route to improve the efficiency of all-polymer solar devices by manipulating charge-transfer excitations.

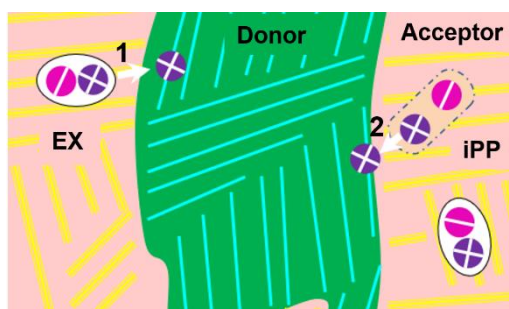


Fig. 1 Possible charge separation channels starting from Frenkel excitons (EX) or charge-transfer states (iPP).

Keywords: organic solar cell; charge transfer state; charge separation; two-dimensional electronic spectroscopy.

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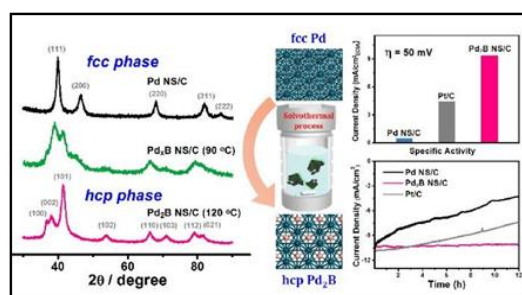
O12 材料催化机理过渡金属基高活性析氢反应

催化材料的理性设计

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水裂解过程中的从质子到氢气转换反应(析氢反应, HER, $2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2$), 是获取清洁氢能的重要手段, 因此该反应被认为是向清洁能源社会发展的重要化学反应。然而, 该反应通常需要以铂(Pt)为基础的材料作为催化剂, 催化剂成本高、长期稳定性不足, 很大程度上限制了其大规模应用。最新的量子化学模拟研究表明, 铂催化剂的高活性原子很大程度上来源于位于催化剂超小纳米颗粒的顶点的高活性位, 而这些顶点的活性位容易在实际反应条件下随着纳米粒子团聚而丢失。为了寻找一种能够在原子紧密堆积的表面上展现出高活性与稳定性的晶体材料, 研究团队通过理论研究, 发现并预测Pd₂B晶体是Pd-B复合物各组分中热力学最稳定的体相结构, 且反应动力学研究表明Pd₂B能够具有比纯铂更高的本征活性, 因此Pd₂B被确定为合适的候选材料。基于上述量子化学理论预测, 研究团队进一步发展了一种简单的溶剂热法合成的碳负载Pd₂B纳米片(NS)。实验表明该Pd₂B纳米片具有超低的HER过电位, 在10 mA cm⁻²电流密度下过电位仅为15.3 mV, Tafel斜率为22.5 mV/Dec, 交换电流密度(j₀)达到2.84 mA cm⁻²。实验还表明该金属硼化物在酸性条件下具有创记录的高本征活性, 比商业化的Pt/C催化剂高约2倍, 并且在反应条件下具有很高的稳定性, 在起始电流密度为j = 10 mA cm⁻²条件下恒压工作12 h后仍保留了97.6%的活性。理论研究结果表明合成过程中, 从纯Pd的面心立方堆积(fcc)结构到六方密堆积(hcp)结构的逐层相变以及后续的B原子的插入是Pd₂B生成的决速步骤, 研究人员采用的溶剂热方法则有效加速了该过程。理论计算表明, hcp晶格形成后的次表面B和晶格膨胀对提升材料的催化活性起着关键作用。该工作为进一步探索这类稳定的金属硼化物材料的催化性能铺平了道路。

Fig. 1 HCP Pd₂B as Superactive Hydrogen Evolution Reaction Catalyst

关键词: 非均相催化; 析氢反应; 密度泛函理论

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O13 Novel Endohedral Fullerene Ions Observed in a FT ICR MS

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For many years, encapsulating different atoms or molecules inside fullerenes is a very interesting and challenging task for chemists. Besides the curiosity of scientists, the unique properties and application potentials of these novel materials are also great motives for such studies. By now, efforts have been greatly devoted to encaging metallic clusters and some small molecules including H₂O into fullerenes to form different endohedral fullerenes. These species also provided us a valuable model to understand how the nanoscale confinement influences the properties of the enclosed species. Using the method of laser ablation mass spectrometry with a FT ICR MS, we recently have observed some new and interesting endohedral fullerene ions. For example, mass spectrometric proofs of fullerenes encaging ionic bonds were observed for LuCl@C₉₀ and LaCl@C₉₀. DFT calculations were also performed for these species, and their interesting properties and the cage effects on the ionic bonds are also discussed.

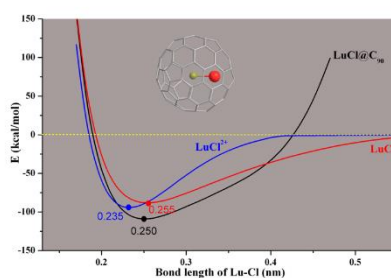


Fig. 1 Potential curves of LuCl²⁺, LuCl, LuCl@C₂(99917)-C₉₀

Keywords: endohedral fullerene; laser ablation; mass spectrometry; ionic bonds; ions

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O14 基于远/中红外多光子解离红外光谱的金团簇和富勒烯-钒团簇 阳离子的结构与性质研究

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团簇是介于单个原子或分子和宏观物质之间的原子分子聚集体，可以看作是凝聚相物质的初生态。解析和阐明具有特定尺寸和组成的团簇的结构与性质，对认识和理解物质微观结构与功能及其演化具有重要意义。红外光解离(infrared photodissociation, IRPD)光谱通过测定团簇的振动结构，可以反映团簇原子间的连接方式、电荷分布和成键性质等信息，是一种有效的表征气相团簇的方法。最近，我们利用荷兰自由电子激光器实验用户中心(FELIX)产生的烯-钒团簇(远红外和中红外波段的红外光(100-1600 cm^{-1}))，通过红外多光子解离(IRMPD)技术得到了金团簇(Au_n^+ , $n \leq 9$)和富勒烯-钒团簇($\text{C}_{60}\text{V}_n^+$, $n \leq 10$)阳离子的红外光谱。结合量子化学理论计算，我们指认了这些团簇的几何结构和键合特征，确认了金团簇阳离子从二维平面(2D)结构向三维立体(3D)结构转变的尺寸，以及钒原子在 C_{60} 富勒烯表面的结合位置、簇合性质及其磁性变化。

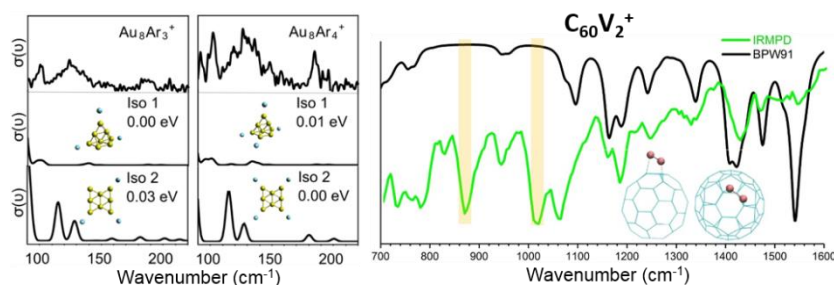


Fig. 1 The IRMPD spectra of Au_8^+ and $\text{C}_{60}\text{V}_2^+$ from experiments and theory as well as their structures

关键词: 红外多光子解离; 自由电子激光; 金团簇; 富勒烯-钒团簇

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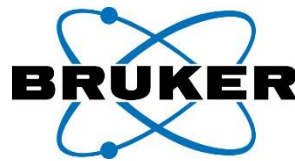


会议笔记



支持单位

主赞助商



Chinese Journal of Chemical Physics

赞助商



METTLER TOLEDO

