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清华大学

Tsinghua University

原子分子纳米科学研究中心
(原子分子纳米科学教育部重点实验室)

Center for Atomic and Molecular Nanosciences

二〇一一年报

2011 Annual Report

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国家科学与技术部
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中心围绕着“原子分子测控科学实验平台”进行建设；该科学实验平台包括“中心激光装置”，“原子分子超灵敏探测装置”，“原子级分辨扫描探针显微装置”，“时空分辨多光子成像-光学相干层析装置”，“细微结构制备装置”，“远场-近场光学显微装置”以及“原子分子模拟装置”等。同时以这些装置为基础，进行纳米科学基础研究；即原子分子层次超灵敏探测、超灵敏识别、操纵和控制技术的基础研究。中心总共 12 位成员。下面列举 2011 年度的研究工作进展。

原子分子超灵敏探测研究部

主任：马万云 王力军

成员：莫宇翔 戴星灿

课题组 A (马万云):

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1、用飞秒激光双光子荧光成像技术，实时动态观测了小鼠早期胚胎 1-2、2-4、4-8 细胞的卵裂过程。[[MWY-1101](#)]

2、用飞秒激光双光子荧光成像技术，研究了衰老因素对小鼠卵母细胞体外成熟过程中 DNA 甲基转移酶表达的影响。观测到衰老引起四种 DNA 甲基转移酶的三维空间表达模式改变（指表达部位与强度）。[[MWY-1102](#)]

3、用实时荧光成像技术，研究了 GSNO 诱导小鼠胸腺细胞凋亡早期胞内游离钙离子浓度与线粒体膜电位变化间关系。观测到胞内游离钙离子浓度变化最快时间点总先于线粒体膜电位变化时间点，这一结果支持钙超载导致线粒体损伤的凋亡模型。[[MWY-1103](#)]

课题组 B (莫宇翔):

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1、利用速度成像技术和四波混频产生 XUV 光技术，我们研究了 H₂S 分子在能量为 15.506, 15.366, 和 15.245 eV 的离子对解离动力学。测量了 $\text{H}_2\text{S} \xrightarrow{\text{XUV}} \text{SH}^-(X^1\Sigma^+, v) + \text{H}^+$ 中光解产物 H⁺ 的速度成像，获得了 SH⁻ 振动态的强度分布和振动态分辨的角分布。用在 CASSCF/6-311++g(3df) 水平上的从头计算方法，我们对离子对态进行了理论计算，得到了离子对态的平衡结构几何参数和有关的势

We have been setting up the “atomic and molecular scientific experiment platform” which consists of “laser system”, “atomic and molecular ultrasensitive detection system”, “high-resolution scanning probe microscope system”, “spatial & temporal resolved multi-photon image-optical coherent tomography system”, “nano fabrication system”, “far-field and near-field optical microscope system” and “atomic and molecular simulation system” etc.. Based on the systems, we(i.e., total 12 members) have carried out some basic researches in nanosciences; namely, ultrasensitive detection, ultrasensitive recognition, manipulation and control of atoms and/or molecules. Some progresses in 2011 are reported as follows.

Division of Atomic & Molecular Ultrasensitive Detection

Directors: Wan-Yun Ma Li-Jun Wang

Members: Yu-Xiang Mo Xing-Can Dai

Group(A) (Wan-Yun Ma):

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The researches include:

1. Mouse zygotes are widely used in developmental biology and transgenic animal research. Two-photon laser scanning microscopy (TPLSM) is particularly useful in four-dimensional observation of big and thick biological samples, such as mouse embryo. The early mouse embryo development from zygote to 8-cell stage compaction was observed in real-time by stages using TPLSM in this paper. During our experiment, several scanning parameters were optimized in different development stages. The initial cleavages of mouse embryo, from the zygote to 2-cell, 2-cell to 4-cell, 4-cell to 8-cell, and the compaction at 8-cell stage were observed. During the first stage, localized intracellular calcium elevation along with the cleavage furrow and the asymmetric zygote cytokinesis was detected. The relation between the asymmetry and the location of the second polar body was investigated. The rotational cleavage of mouse embryo was also observed

能曲线。结合实验与理论计算,我们认为H₂S离子对解离是一个预解离过程,其机制为:分子从基态跃迁到收敛于H₂S⁺(2²A')的里德堡态,里德堡态与离子对态6A'发生相互作用,然后由6A'解离得到碎片离子SH⁻和H⁺。[\[MYX-1101\]](#)

2、基于透热模型发展出一套处理电子-自旋-振动耦合的高精度程序包,结合从头计算法研究了CH₃O自由基中强电子-振动相互作用和自旋-轨道耦合效应,成功地解释了CH₃O的高分辨自由基光谱实验数据。结果表明:CH₃O中存在较强的电子-振动相互作用和自旋-轨道耦合效应;高精度透热模型可以很好地解释电子-振动相互作用引起的振动高分辨光谱。对比理论结果和实验数据,讨论了CASPT2和MRCI对处理CH₃O自由基体系光谱带来的影响。[\[MYX-1102\]](#)

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2011年,精密测量联合实验室在时间频率领域的多个研究方向均有重要进展。例如,我们实现了原子时信号的高稳定度光纤传输,达到了10⁻¹⁸的水平,成果经专家组鉴定达到了世界领先水平。另外,激光冷却可搬运镉离子微波频标(973)系统搭建完毕,并已获得窄线宽Ramsey信号,经闭环锁定有望实现高稳定度的可搬运频标。[\[wlj-1101,wlj-1102,wlj-1103-wlj1109\]](#)

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2011年里我主要完成了和正在完成以下工作[\[dxc-1101-dxc1103\]](#):

1、在碱金属双原子分子的高激发态的研究中,我们用光学双共振的方法观测并归属了Rb₂的2IΠg态,共观察到了该电子态的254能级,并用同位素效应归属了它们的振动能级。我们得到了该态的分子常数和RKR势能曲线。这是Rb₂中观测到的第一个高激发g态。相关文章已经写作完毕,正准备投稿。我们还购买了另一台Toptica的连续激光器,这台激光器的波长和我们现有的激光器不同。我们将继续研究Rb₂其它的高激发电子态,尤其是我们感兴趣的高激发三重态。

in the experiment. These results would be helpful to further research on mammalian embryonic development. [\[MWY-1101\]](#)

2. The effects of maternal aging on the localization of DNA methyltransferases were evaluated during mouse oocyte maturation using fluorescence staining. And we conclude that maternal aging affects the cytoplasmic-to-nuclear trafficking of DNA methyltransferases in mouse oocytes during the time from germinal vesicle breakdown to metaphase I. [\[MWY-1102\]](#)

3. A fluorescence microscopy imaging technique was applied to observe the kinetic changes of intracellular Ca²⁺ concentration ([Ca²⁺]_i) and mitochondrial membrane potential (ΔΨ_m) in single thymocytes during the early stage of S-nitrosoglutathione (GSNO)-induced apoptosis. The kinetic features of [Ca²⁺]_i and ΔΨ_m were quantitatively analyzed and compared by fitting the fluorescence intensity data. The mathematical parameter, inflection point which indicated the time point when [Ca²⁺]_i or ΔΨ_m changed the most rapidly, was proposed to analyze the fitting curve. The results revealed that the inflection point of [Ca²⁺]_i always appeared prior to that of ΔΨ_m during apoptosis induced by a certain GSNO concentration. Both the [Ca²⁺]_i and ΔΨ_m changed in a GSNO concentration-dependent manner. Another parameter, half-max effect point also employed and displayed the similar results. Such quantitative analyses of real-time observations at the single-cell level are useful for interpreting the sequence of the biological events operating in GSNO-induced thymocyte apoptosis. [\[MWY-1103\]](#)

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1. The H⁺ velocity map images from the ion-pair dissociation of H₂S+hν→SH⁻($\tilde{X}^1\Sigma^+, \nu=0,1$)+H⁺ have been measured at the excitation energies 15.259, 15.395 and 15.547 eV, respectively. The experimental results show that most of the available energies are transformed into the translational energies. The angular distributions of the fragments

2、与薛平教授和中科院钟志萍教授合作的冷原子实验中，我们重新测量了 Rb 原子 $5P_{3/2}$ 态的电离截面，测量结果要比以前其它小组的测量更为精确。该实验结果的相关文章已经投稿，正处于审稿中。我们还在继续研究由于电离光电离冷原子后造成的冷原子团的温度的变化。

3、我们与姜开利教授合作，试图用两束激光激发碳纳米管中的声子。两束激光的频率差即所要激发的声子的频率用声光调制器和电光调制器控制。虽然还没有很好的实验结果但实验还在继续进行中。

原子分子超灵敏识别研究部

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2011 年“光学相干 CT 研究”的年度工作进展报告

研制了新型的基于分波前的光学相干 CT 成像，可以优化系统的信噪比。利用不同的波前作为样品和参考光，研究了不同配比的样品和参考光的实验系统信噪比，并和理论值对比获得了很好的一致性。目前系统总光功率 7.5mW 的 8% 作为参考光，可获得高达 115dB 的信噪比，并进行了实时成像。鲜红斑痣光学相干 CT 在实际临床病例诊断中，成功获得应用，对病理研究、临床诊断及术后效果评价方面具有很好的应用价值。进一步的图像识别及参数提取研究在进行中。[[XP-1101](#)]

原子分子控制研究部

主任：薛其坤 张新荣

成员：王亚愚 李景虹

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在拓扑绝缘体电子结构以及铁基超导体超导机制研究方面，取得了重大进展。[[xqk-1101-xkq-1113](#)]

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点文献号跳至文献清单,点文献跳至全文。

$SH(\tilde{X}^1\Sigma^+, \nu=0)$ indicate that the dissociation occurs via pure parallel transition with limiting anisotropy parameter of +2. This suggests that the ion cores of the excited Rydberg states predissociated by the ion-pair states have linear geometries. The geometries and electronic structures of linear $H_2S^+(1^2\Sigma_g^-, 1^2\Delta_g$ and $1^2\Sigma_g^+)$ have been calculated employing the quantum chemistry calculation method at the CASPT2/avqz level. Combining the experimental and theoretical results, it is proposed that the B band in the photoelectron spectrum of H_2S should have contributions from some linear $H_2S^+(1^2\Sigma_g^-, 1^2\Delta_g$ and $1^2\Sigma_g^+)$ in addition to $H_2S^+(1^2B_2)$ that has a bent equilibrium geometry. The electronic structures for the ion-pair states have been calculated at the CASSCF/avtz level, which indicates that the equilibrium geometries of the ion-pair states have bent geometries. [[MYX-1101](#)]

2. We present an *ab initio* study of the spin-vibronic couplings in $CH_3O(X^2E)$ based on diabatic model. The diabatic potential energy curves were calculated at the level of CASPT2/cc-pvtz. The calculated spin-vibronic energy levels are compared with the experimental data, which indicates that the present calculation has higher accuracy than the previously reported one. [[MYX-1102](#)]

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The Joint Institute of Measurement Science has multiple achievements in time and frequency research area. For example, we have built an accurate time and frequency synchronization system via optical fiber, and achieved the stability of 10^{-18} , which is, according to the assessment of expert group, ranking the world's top level. Also, the portable Cadmium ion frequency standard system has been almost finished, and the Ramsey fringe with narrow linewidth has been demonstrated. After finishing the locking loop, we will realize a portable frequency standard with high stability (2×10^{-14}). [[wlj-1101,wlj-1102,wlj-1103-wlj1109](#)]

1、报道了一种 SP-ICP-MS 分析 DNA 的新方法。将表面修饰特定序列的 DNA 片段进行杂交后，会引起金纳米粒子的聚集，使得纳米粒子计数减少，信号峰提高，据此可以对特定 DNA 序列进行分析测定。该方法扩展了 ICP-MS 的应用范围，为元素分析仪器迈进生命科学领域提供了新思路。[ZXR-1101]

2、提出一种基于阵列传感模式进行蛋白质识别的新方法。该阵列由不同催化活性的纳米材料组成，一种蛋白质能够在阵列上形成一个特定的指纹图谱，因此能够获得识别。该传感阵列还可以扩展到识别不同的细胞。论文初步探索了从正常细胞中识别癌变细胞的可能性。[ZXR-1102]

3、合成了一种金-蛋白质荧光纳米簇。蛋白质是辣根过氧化物酶，由于其具有催化活性，因此，当体系中含有过氧化氢时，该酶能够催化过氧化氢氧化纳米簇自身而导致荧光猝灭。采用这一方法，能够对样品中所含的过氧化氢进行测定。该方法为这类荧光纳米材料的功能化和分析应用提供了一种新思路。

[ZXR-1103]

4、建立了一种热致发光识别蛋白质的新方法。采用所研制的热致发光仪器对蛋白质的亚型和不同折叠状态进行了识别。结果发现，三种不同的白蛋白包括人血清白蛋白、牛血清白蛋白以及猪血清白蛋白能够很好的区分。不同变性状态下的白蛋白也获得了较好的区分，证明这是一种新的有效分析蛋白质的方法。[ZXR-1104]

5、设计了一种简单的低温等离子体质谱离子源，该离子源能够对所研究的多种环境污染物（VOCs）产生单一的分子离子峰，因此有可能实现不经色谱分离直接对复杂的混合样品中各种 VOCs 进行测定。由于这种离子源功率较低，且不需要惰性气体，能够直接在空气条件下工作，因此运行方便且成本较低，比较适合小型质谱作为离子源工作。

[ZXR-1105]

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我们的工作有[wyy-1101-wyy-1105]:

1、研究了 MBE 生长的拓扑绝缘体薄膜的输运性质随薄膜层厚（维度）的变化，发现其磁阻呈现典型的弱反局域化行为，但电阻呈

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In 2011, I have been working on the following projects[[dxc-1101](#)-[dxc1103](#)]:

1. In the study of the highly-excited Rydberg states of alkali molecular dimmers, we used the optical-optical double resonance method to observe and assign the $2^1\Pi_g$ state of Rb_2 . Totally 254 energy levels were observed and the absolute vibrational number is assigned with isotope effect. We obtained the molecular constants and RKR potential curve of the state. The manuscript is written and ready to submit. We have also purchased another diode laser from Toptica. This diode laser will allow us to study other highly-excited Rydberg states of Rb_2 , especially highly-excited triplet states.

2. In the experiment of cold atoms that is cooperation with Prof. Ping Xue and Prof. Zhiping Zhong, we measured the ionization cross section of the $5P_{3/2}$ level of Rb and the result is more accurate than the results from other groups. The manuscript is submitted and under review. Currently we are studying the temperature change of the cold atoms after the photoionization.

3. We have also cooperated with Prof. Kaili Jiang and try to use lasers to excite the phonons in their nanotube materials. The frequency of the excited phonons is controlled by the acousto-optic or electro-optic modulators. The experiment is going on well.

Division of Atomic & Molecular Ultrasensitive Recognition

Director: Ping Xue

Group(A) (Ping Xue):

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We built a new Wave Front (WD) Division Interferometer Based Optical Coherence Tomography (OCT) for Sensitivity Optimization. Unlike a conventional amplitude division interferometer based OCT, WD OCT utilizes different wave front portions of the light source for sample and reference arm. The system sensitivity as a function of the ratio of light power directed to the two arms is experimentally studied and the

现一种反常的绝缘性行为，且随维度降低绝缘性行为变强。我们认为这是由无序拓扑绝缘体中的电子电子相互作用引起。

2、利用同族、同结构的 Sb_2Te_3 和 Bi_2Te_3 拓扑绝缘体中的不同缺陷类型，通过 MBE 生长的三元合金来调节拓扑绝缘体的能带结构。我们发现在一定的区间，体系可以成为理想的拓扑绝缘体，体态基本完全绝缘，而表面态的行为呈现二维简并度为一的狄拉克费米子行为。

3、利用扫描隧道显微镜 (STM) 研究了 LaOFeAs 铁基超导体母体的实空间电子结构，发现了一个明显的二维表面电子态，其电子驻波形式呈现二次对称性，与在其他铁基超导体的母体行为相似，因此可能是铁基超导体母体的共性。

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1、发展高性能锂离子电池已经成为解决能源危机和环境问题的重要途径。结构稳定，理论比容量大的 LiFePO_4 成为高性能动力锂离子电池的重要阴极材料，但其电子传输性能与离子传输能力差影响了进一步的发展。我们通过对 NH_4FePO_4 热处理和稀酸洗涤交替进行，制备多孔纳米片组装成的具有微米球结构的 FePO_4 ，再在室温下用 LiH 还原，以蔗糖为碳源真空条件下原位包覆碳层，成功制备了原位碳包覆的 LiFePO_4 多孔纳米片组装微球。结合多孔结构、片状结构、核壳结构以及组装效应，有效地提高了 LiFePO_4 的电子传输性能与离子传输性能，及嵌脱锂稳定性。这种材料作为锂离子电池阴极材料，在 0.1 C ($1\text{ C}=170\text{ mA g}^{-1}$) 放电倍率下容量为 158 mAh g^{-1} ，在 5 C 的放电倍率下容量仍有 85 mAh g^{-1} ；在倍率从 0.1 C 到 5 C 不断变化下的 80 圈充放电循环中，能量效率始终高于 96% ，相比普通纳米颗粒材料，该材料比容量高，循环稳定性好，大倍率放电容量保持率高，适合作为高功率锂离子电池的阴极电极材料。这种制备方法简单、安全、适用面广，还可作为开发其他高性能电极材料的制备方法。 [[ljh-1101](#)]

2、如何实现石墨烯及其衍生物的可控自组装是重要的研究命题。我们结合 DNA 的杂

result found to be well consistent with the theoretical analysis. In our current time-domain WD OCT, we have achieved the system sensitivity as high as 115dB at a total source power of only 7.5mW with 8% to the reference arm. Real-time WD OCT imaging of bio-tissues in vivo is also demonstrated.

OCT Real-time and in situ imaging of the port wine stains patient and supplying surgery guidance for photodynamic therapy treatment prove successful in clinic. OCT is also good for pathology study and treatment assessment. Image recognition and parameter study are in progress. [[XP-1101](#)]

Division of Atomic & Molecular Control

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We made great achievements on the researches of the electronic structure of topological insulators and the superconducting mechanism of iron-based superconductors. [[xqk-1101-xkq-1113](#)]

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1. In this paper, we have demonstrated a novel method to detect special sequence DNA targets in one-step homogeneous hybridization solutions with single-NP detection. The DNA targets can be detected at 1 pM by using AuNP probes, which increase the sensitivity by three orders of magnitude over that of colorimetric methods, without any signal amplification process. Additionally, ICP-MS is able to detect NPs without any special requirements for optical and electrochemical properties, so an expanding range of NPs such as biological tags can be applied. [[ZXR-1101](#)]

2. We report a sensor array based on nanomaterial-assisted chemiluminescence (CL) for protein sensing and cell discrimination. We have found that the CL efficiencies are improved to varied degree for a given protein on cell line on catalytic nanomaterials. Distinct

交配对作用，成功实现了石墨烯氧化物的层层自组装。原子力显微镜，X 射线衍射和透射显微镜有力证明了组装体的层状结构。同时，利用动态光散射和荧光各向异性技术研究了组装的过程，证明了 DNA 在组装过程中的引导和控制作用。另外，利用 DNA 互补配对的特性，结合动态光散射技术，利用该组装过程实现了目标 DNA 的高灵敏度的选择性检测。该工作提供了二维材料的层状组装的普适性方法，在生物传感，医学诊断，材料组装，器件构造上具有潜在的意义。[[ijh-1102](#)]

3、石墨烯是由周期性排列的碳六元环组成的蜂窝状点阵结构二维平面材料，它只有一个分子的厚度，可以包裹成零维的富勒烯结构，卷曲成一维的碳纳米管结构或者层层堆积成三维的石墨结构，石墨烯被认为是构成各类石墨结构材料的基本组成单元。除了独特的二维平面结构，石墨烯还具有其他一些奇异的电子及机械性能，从而吸引了物理学，化学和材料学等领域科学家们的广泛关注。我们选择性地评述了近期有关石墨烯及其氧化物在生物化学和生物技术方面的研究进展，阐述了通过物理或化学方法实现对于石墨烯材料的生物功能化修饰和应用实例；利用石墨烯材料的荧光淬灭效应，可以实现基于荧光共振能量转移机理的生物传感器的设计和制备；以及基于石墨烯及其氧化物等复合材料在活细胞体系中的检测，成像和靶向药物释放的研究。进一步提出了石墨烯材料在迅速发展的生物技术应用领域中存在的问题和面临的机遇与挑战。[[ijh-1103](#)]

4、成功制备了一种石墨烯修饰新型玻碳电极，研究了鲁米诺在该修饰电极上的电化学发光行为。研究表明，该石墨烯修饰电极有利于活性氧的形成，使得鲁米诺工作电位为 0.05 V (vs. Ag/AgCl) 时，即可产生非常强的阴极电化学发光。利用石墨烯大的比表面积和优异的电子传递能力，将一抗修饰到该石墨烯修饰电极表面，再采用金纳米棒负载葡萄糖氧化酶和二抗对鲁米诺电化学发光进行催化放大，发展了一种多重信号放大传感技术，成功地构建了一种电位低、灵敏度高、选择性好的夹心结构电化学发光免疫传感器。该传感器可用于癌症标记物-前列腺抗原的高灵敏分析检测，检测限为 8 pg mL^{-1} ，线性范围为 10 pg mL^{-1} 到 8 ng mL^{-1} ，具有很

CL response patterns as "fingerprints" can be obtained on the array and then identified through linear discriminant analysis (LDA). The sensing of 12 kinds of proteins at three concentrations, as well as 12 types of human cell lines among normal, cancerous, and metastatic, has been performed. Compared with most fluorescent or colorimetric approaches which rely on the strong interaction between analytes and sensing elements, our array offers the advantage of both sensitivity and reversibility. [[ZXR-1102](#)]

3. In this work, we report a new strategy to construct enzyme functionalized fluorescent gold nanoclusters via a biomineralization process for the detection of hydrogen peroxide. Horseradish peroxidase (HRP) was used as a model functional template to direct the synthesis of fluorescent gold nanoclusters (Au NCs) at physiological conditions to form HRP-Au NCs bioconjugates. We found that the fluorescence of HRP-Au NCs can be quenched quantitatively by adding H_2O_2 , indicating that HRP enzyme remains active and enables catalytic reaction of HRP-Au NCs and H_2O_2 . This study would be potentially extended to other functional proteins to generate dual functional nanoclusters and applied to real time monitoring of biologically important targets in living cells. [[ZXR-1103](#)]

4. We improve traditional TCL assays using the assistance of catalytic nanomaterials and construct a nanomaterials array for the discrimination of three subtypes of proteins (albumin from human serum, bovine serum and porcine serum). With the assistance of catalytic nanomaterials, TCL signals of different protein samples are distinct due to the diverse catalytic activities of the nanomaterials and characteristics of proteins. In the blind test, 24 unknown samples randomly chosen from these albumins were all assigned to the accurate groups. This improved TCL assay with reversible response and simple instrumentation can offer high differentiability and sensitivity. [[ZXR-1104](#)]

5. A simple-structure, low-power, and low-cost low temperature plasma (LTP) ionization source, coupled with mass spectrometry, for the online detection of indoor volatile organic compounds (VOCs) has been constructed in this work. Air, instead of noble gases, was

好的稳定性和重现性。利用该传感器，成功地实现了对 10 个病人血清中前列腺抗原的精确检测，具有很高的可靠性，该传感器在癌症标记物临床筛选、实时现场疾病诊断和检测中具有很好的应用前景。[[ljh-1104](#)]

5、石墨烯是一个零带隙的半金属材料，因此为了将石墨烯的应用扩展到光电子与光子方面，打开石墨烯的带隙是非常重要的一个途径。现在打开石墨烯带隙的方法有较多缺点，比如只能打开很小的带隙，需要使用有害且环境苛刻的化学氧化，或需要昂贵复杂的化学气相沉积技术。为此，我们发展了一种在任意条件下、环境友好、高效、可以大量制备的化学方法来合成氟化石墨烯半导体的方法。该方法，离子液体被用作唯一的化学试剂去剥离商业可获得的氟化石墨，来获取单层或者少层的氟化石墨烯。实验结果与理论计算表明，氟化石墨烯的带隙依赖于 F 原子的含量与其构象，可以在很宽的范围内调节石墨烯能带。[[ljh-1105](#)]

6、合成了一种新型的聚合离子液体修饰的石墨烯 (poly(ViBuIm+Br⁻)-G) 纳米复合材料。利用 FTIR、Uv-vis 以及 TEM 等方法，对该复合材料的制备过程以及形貌特点等进行了表征。由于聚合离子液体的修饰，这种纳米复合材料不但可以以单独的纳米片形式均匀分散于水溶液中，形成稳定的悬浊液，而且可在水溶液中呈现较强的正电荷。因此，通过自组装方法，这种正电荷的复合材料可在温和条件下，在玻碳电极表面上实现对负电荷的葡萄糖氧化物酶 (GOD) 的固载，进而构筑了新型化学修饰电极

(GOD/poly(ViBuIm+Br⁻)-G/GC 电极)。由于聚合离子液体以及石墨烯均具有优良的性质，poly(ViBuIm+Br⁻)-G 可为固载的 GOD 提供一个生物相容且导电的微环境，从而使 GOD 能够实现与电极的直接电子传输。利用 GOD/poly(ViBuIm+Br⁻)-G/GC 电极，还可实现对葡萄糖的检测。实验结果表明，该修饰电极对葡萄糖的检测具有较宽的线性范围和优良的稳定性。因此，这种具有独特性质的纳米复合材料可被用于构筑新型无媒介体的电化学酶传感器。[[ljh-1106](#)]

7、通过原位生长机制能够原位实现纳米金颗粒的成核生长和石墨烯氧化物的化学还原，从而通过一步法成功制备负载纳米金颗粒的

employed as the discharging and carrier gas. A custom-built AC high-voltage power supply was used. This LTP source is a soft ionization source. The initial performance of the ionization source has been evaluated by ionizing samples including alcohols, ketones, aldehydes and aromatics. These compounds cover most of the common air pollutants concerning people's health. Further work has been conducted to confirm the detection feature of this source. The results are promising enough to ensure the novel LTP ionization source as an effective tool for the online detection of indoor VOCs. [[ZXR-1105](#)]

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Our results include [[wyy-1101-wyy-1105](#)]:

1. We study the transport properties of MBE-grown topological insulator thin films and their evolution with film thickness. We found that the magnetoresistance exhibits the characteristic behavior of weak antilocalization, but the resistance shows an unconventional insulating behavior at low temperatures. We argue that this is due to the electron-electron interaction effect in disordered topological insulators.

2. We utilize the different types of defects in isostructural isovalent Sb₂Te₃ and Bi₂Te₃ topological insulators to tune the band structure of topological insulators. We found that the MBE-grown Bi₂-xSb₂Te₃ ternary topological insulator alloys show the ideal topological insulator electronic structure in certain regime of doping. The bulk becomes a true insulator and the surface states behave like two dimensional Dirac fermions with degeneracy 1.

3. We use scanning tunneling microscopy (STM) to study the local electronic structure of LaOFeAs, the parent compound of iron based superconductors. We found that there is a two dimensional surface states on the LaO surface, and the electron standing wave patterns show two-fold symmetry. This is consistent with previous STM work on 122 type parent compounds, indicating that it is a common feature of the parent compound of iron based superconductors.

化学还原石墨烯纳米片层复合体。该方法巧妙地利用了高分子聚电解质 PDDA

(poly(diallyldimethylammonium chloride)) 的电荷效应, 其不仅作为纳米金颗粒在石墨烯氧化物表面原位生长的稳定剂, 还通过静电吸附自组装的方法进一步将乙酰胆碱酯酶温和均一地固定在纳米金颗粒表面, 得到了酶负载的纳米金/化学还原石墨烯生物功能性材料。使用 TEM, XRD 和 XPS 等方法对材料进行表征, 证明可用于制备高负载量, 高均一度的纳米金石墨烯复合体。根据对氧磷 (paraoxon) 对乙酰胆碱酯酶的高选择性抑制机制, 利用纳米金颗粒的电催化活性以及石墨烯纳米片的高比表面积和电导率, 将此生物功能性材料用于制备高灵敏有机磷电化学传感器。实验结果表明, 基于该方法制备的电化学传感器能够响应低至 0.1 pM 的痕量对氧磷样品, 检测限低于以往关于有机磷电化学传感器报道。[[ljh-1107](#)]

8、发展一步水热非模板法合成了 SnO₂ 八面体颗粒自组装多孔微球。SEM 及 TEM 分析表明, 这种多孔微球由宽约 40 nm, 长约 60 nm, 暴露 (221) 晶面的 SnO₂ 八面体颗粒构成。把这种结构用于锂离子电池, 发现在放电电流为 500 mA g⁻¹ 的高倍率情况下, 循环 50 次后, 其仍然能保持 690 mA g⁻¹ 的容量。这种高容量及容量保持性能, 应该归因于这种优越的纳米结构: (221) 面的 SnO₂ 颗粒有利于脱嵌 Li 反应, 因而容量高; 自组装多孔结构能够缓解充放电过程中的体积膨胀, 因而循环性能好。[[ljh-1108](#)]

9、在水溶液中, 200–210 °C 反应条件下, 简单、温和地合成了高纯度、高结晶、热稳定性好的具有层状结构的 Ni₃Si₂O₅(OH)₄ 多壁纳米管。这种材料中, 用 NaBH₄ 可以可控地原位还原层与层之间的镍原子, 生成单质镍纳米晶, 从而赋予了材料可控的磁性。另外, 将这种具有层状结构的 Ni₃Si₂O₅(OH)₄ 多壁纳米管用于锂离子电池负极材料研究中, 其层状可以提供良好的锂离子动力学传输性能。因而, 该材料在 20 mA g⁻¹ 倍率下, 21 次嵌脱锂循环后, 储锂比容量仍有 226.7 mA h g⁻¹。在此基础上, 将该材料进行热处理 (600 °C, 4 小时) 或者还原 (180 °C, 10 小时), 其嵌脱锂容量被分别提高至 277.2 mA h g⁻¹ 和 308.5 mA h g⁻¹。[[ljh-1109](#)]

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1. We have successfully developed a facile method to synthesize the hierarchical LFP/C NMs with the advantages of simple synthetic steps, facile control of the nanoplate building block, easy repetition of the process, and the possibility to carry out large-scale synthesis. Such a unique hierarchical structure provides favorable transport kinetics for both Li⁺ ions and electrons. The results clearly demonstrate that the hierarchical LFP/C NMs electrode has superior lithium-storage capability with a stable cycle life and exceptional rate capability, indicating their potential application as a serious candidate for the development of high-performance, advanced lithium batteries directed to the hybrid vehicle and electric vehicle markets. Finally, this method can be easily extended to fabricate other hierarchical structural materials. [[ljh-1101](#)]

2. Controlled graphene or its derivatives' assembly is of growing interest in many areas. However, achieving control over their assembly into precise and predictable architectures has been challenging and is still a bottleneck to their utilization. Herein, we report for the first time the use of DNA hybridization for the controllable assembly of a graphene nanosheet. Moreover, with the help of dynamic light scattering technique, we extended the above studies by exploiting the DNA-graphene dispersed sheets as highly ultrasensitive detection of oligonucleotides for the fabrication of a novel biosensing strategy, which shows high sensitivity and excellent selectivity. This work will show a new general route to graphene-based lamellar composite materials and would bring about advances in the research of graphene-based biofunctional materials for specific applications in biodiagnostics, nanoelectronics, and bionanotechnology. [[ljh-1102](#)]

3. Graphene is the basic building block of 0D fullerene, 1D carbon nanotubes, and 3D graphite. Graphene has a unique planar structure, as well as novel electronic properties, which have attracted great interests from scientists. This review selectively analyzes current advances in the field of graphene bioapplications. In

10、使用温度敏感聚合物凝胶聚异丙基丙烯酰胺 (PNIPAm), 物理吸附聚丁二炔

(PPCDA) 囊泡。实验中观察到, 对于吸附于温敏凝胶中的聚丁二炔囊泡, 温度变化更易于引起其蓝色-红色转变。与水溶液中自由分散的囊泡相比, 转变温度从 59~63°C 降低到 52~55°C。对于聚丁二炔囊泡温敏颜色转变过程, 使用紫外-可见光谱, 拉曼光谱, 示差扫描量热法等多种手段进行详细研究。根据温度敏感聚合物凝胶在其最低临界转变温度 (LCST) 发生的溶胀-收缩相变机理, 并结合扫描电子显微镜证据, 推断温度敏感聚合物凝胶在发生相变时, 在凝胶内部产生的静压力附加给聚丁二炔囊泡部分机械力, 进而引起了颜色转变, 使得在升温过程中, 聚丁二炔囊泡能够在较低的温度下, 完成蓝色-红色的转变。实验结果表明, 在聚丁二炔囊泡颜色转变过程中, 其与负载基体在微观和宏观尺度上的相互作用不可忽视; 通过有目的地设计负载基体, 控制基体与聚丁二炔囊泡的相互作用, 可以更好的调控聚丁二炔囊泡颜色转变过程, 扩展其在化学/生物传感领域中的应用。[[ljh-1110](#)]

11、用一步非模板法制备了花状 SnO₂ 纳米球状结构, 并提出了其可能的生长机理。把这种 SnO₂ 纳米球用于气敏传感器, 显示出高的敏感性和快的反应恢复时间。同时将这种 SnO₂ 纳米结构用于锂电池负极材料研究, 研究了不同反应时间产物的电池性能, 结果表明, 6 小时的样品具有最好的锂电池性能, 在 100 圈循环后容量仍能保持 570 mA g⁻¹。通过分析, 我们认为优越的气敏性能主要取决于这种多级结构有利于气体扩散, 以及大的比表面积有利于 SnO₂ 材料和气体相互作用。同时这种 3D 结构有利于减轻 SnO₂ 负极材料在脱嵌 Li 过程中的体积膨胀, 保持了结构稳定性, 因而循环性能好。[[ljh-1111](#)]

12、电化学 DNA 传感器由于其灵敏度高、选择性好、轻便、低成本、低能耗等优势受到广泛的关注, 在基因测序和疾病诊断等方面具有重要的应用价值。石墨烯由于其独特的二维晶体碳纳米结构和电学性质引起了广泛的关注。其二维结构和大的比表面积使得它可以很容易地与其它零维、一维纳米材料构建新型先进复合纳米结构材料, 并具有更高的电子传递效率, 为发展性能优异的电化

particular, the biofunctionalization of graphene for biological applications, fluorescence-resonance-energytransfer-based biosensor development by using graphene or graphene-based nanomaterials, and the investigation of graphene or graphene-based nanomaterials for living cell studies are summarized in more detail. Future perspectives and possible challenges in this rapidly developing area are also discussed. [[ljh-1103](#)]

4. In this work, we report a cathodic electrogenerated chemiluminescence (ECL) of luminol at a positive potential (ca. 0.05 V vs Ag/AgCl) with a strong light emission on the graphene-modified glass carbon electrode. The resulted graphene-modified electrode offers an excellent platform for highperformance biosensing applications. On the basis of the cathodic ECL signal of luminol on the graphene-modified electrode, an ECL sandwich immunosensor for sensitive detection of cancer biomarkers at low potential was developed with a multiple signal amplification strategy from functionalized graphene and gold nanorods multilabeled with glucose oxidase (GOx) and secondary antibody (Ab2). The functionalized graphene improved the electron transfer on the electrode interface and was employed to attach the primary antibody (Ab1) due to its large surface area. The gold nanorods were not only used as carriers of secondary antibody (Ab2) and GOx but also catalyzed the ECL reaction of luminol, which further amplified the ECL signal of luminol in the presence of glucose and oxygen. The as-proposed low-potential ECL immunosensor exhibited high sensitivity and specificity on the detection of prostate protein antigen (PSA), a biomarker of prostate cancer that was used as a model. A linear relationship between ECL signals and the concentrations of PSA was obtained in the range from 10 pg mL⁻¹ to 8 ng mL⁻¹. The detection limit of PSA was 8 pg mL⁻¹ (signal-to-noise ratio of 3). Moreover, the asproposed low-potential ECL immunosensor exhibited excellent stability and reproducibility. The graphene-based ECL immunosensor accurately detected PSA concentration in 10 human serum samples from patients demonstrated by excellent correlations with standard chemiluminescence

学传感器提供了平台。我们利用石墨烯与单链 DNA 之间的非共价吸附作用, 直接将探针 DNA 固定在石墨烯修饰的玻碳电极表面, 利用捕获 DNA 分子、目标 DNA 分子和互补 DNA 链修饰的金纳米粒子的识别和组装, 构建了一个夹心结构的传感器, 并通过纳米金标银染放大技术进行电化学溶出伏安检测, 发展了一种高灵敏、性能稳定的电化学 DNA 传感器。石墨烯大的比表面积提高了捕获 DNA 探针分子负载量, 同时避免了传统的共价接合方法中繁杂的操作手续以及共价固定化 DNA 方法中由于电化学检测过程中电化学氧化带来的测量上的限制。结合银染放大电化学检测技术, 进一步提高了传感器的灵敏度。该方法操作简易且性能稳定, 并成功地应用于单碱基错配 DNA 序列的分析测试。这种基于石墨烯和 DNA-金纳米粒子组装的电化学 DNA 传感器在卫生防疫、临床诊断和公共安全等方面具有广阔的应用前景。[[ljh-1112](#)]

13、提出了结合石墨烯的基体辅助激光解吸电离时间飞行质谱法, 用于环境污染物中的疏水化合物的快速分析。传统基质的 MALDI-TOF MS 在分析低极性化合物会遇到一些困难。但该研究表明, 石墨烯对疏水化合物具有高脱附和电离作用, 且没有小碎片产生, 同时具有一定的定量能力。研究还发现, 石墨烯的离子化信号的强度和被分析物的苯环个数有关, 苯环越多, 离子化信号越强, 这与石墨烯和化合物间的 π - π 重叠强度有关。将该技术应用于实际样品 (如河水) 的快速萃取和分析, 结果表明其具有很强的检测能力, 最低检测限低至 100 nM。因此, 以石墨烯为基底的 MALDI-TOF MS 的技术具有重要的应用价值。[[ljh-1113](#)]

14、多级 TiO_2 纳米结构能有效地提高染料吸附量、光散射能力, 并具有优越的载流子分离及运输能力, 因而是制备染料敏化太阳能电池的一个理想纳米结构。我们先应用水热法在 FTO 导电玻璃基底上制备出 TiO_2 纳米棒阵列, 然后以其为种子, 制备出垂直生长具有分叉结构的树状多级 TiO_2 纳米结构。把这种多级结构组装成染料敏化太阳能电池, 在只有 3 微米的长度下, 取得了 10.05 mA cm^{-2} 的光电流, 光电转换效率能达到 3.75%, 比纯的 TiO_2 棒阵列增大了 3 倍。这种优良的

immunoassay. The results suggest that the as-proposed graphene ECL immunosensor will be promising in the point-of-care diagnostics application of clinical screening of cancer biomarkers. [[ljh-1104](#)]

5. The bandgap opening of graphene is extremely important for the expansion of the applications of graphene-based materials into optoelectronics and photonics. Current methods to open the bandgap of graphene have intrinsic drawbacks including small bandgap openings, the use hazardous/harsh chemical oxidations, and the requirement of expensive chemical-vapor deposition technologies. Herein, an eco-friendly, highly effective, low-cost, and highly scalable synthetic approach is reported for synthesizing widebandgap fluorinated graphene (F-graphene or fluorographene) semiconductors under ambient conditions. In this synthesis, ionic liquids are used as the only chemical to exfoliate commercially available fluorinated graphite into single and few-layer F-graphene. Experimental and theoretical results show that the bandgap of F-graphene is largely dependent on the F coverage and configuration, and thereby can be tuned over a very wide range. [[ljh-1105](#)]

6. A novel polymeric ionic liquid functionalized graphene, poly(1-vinyl-3-butylimidazolium bromide)-graphene (denoted as poly(ViBuIm+Br⁻)-G), was synthesized. FTIR, UV-vis spectra and TEM were used to characterize the formation of as synthesized nanocomposites. Due to the modification of the polymeric ionic liquid, poly(ViBuIm+Br⁻)-G can not only be dispersed well in aqueous solutions to form a homogeneous colloidal suspension of individual nanosheets, but also exhibit a strong positive charge. Based on self-assembly, the negatively charged glucose oxidase (GOD) was immobilized onto the poly(ViBuIm+Br⁻)-G to form a GOD/poly(ViBuIm+Br⁻)-G/glassy carbon (GC) electrode under mild conditions. With the advantage of both poly(ViBuIm+Br⁻) and graphene, poly(ViBuIm+Br⁻)-G can provide a favorable and conductive microenvironment for the immobilized GOD and thus promote their direct electron transfer at the GC electrode. Furthermore, the GOD/poly(ViBuIm+Br⁻)-G/GC electrode

性能主要源于其优越的纳米多级结构。[[ljh-1114](#)]

15、电化学 DNA 传感器具有高灵敏度、特异性、可携带性，同时易与微电子器件集成的能力，日前引起了人们广泛的兴趣。很多策略被用来设计高灵敏度与特异性的电化学 DNA 传感器，例如使用金属纳米颗粒，磁性纳米颗粒，半导体纳米颗粒与碳纳米材料（尤其纳米碳管），并在基因分析、临床诊断、环境与食品安全方面的进行了大量的应用研究。在该综述中，我们对电化学 DNA 传感器的挑战与机遇进行了简短的评述。[[ljh-1115](#)]

16、发展了一种新的基于石墨烯/聚噻吩纳米复合材料，应用于光电化学池研究光电转换性能。首先通过吡啶酸修饰得到可以溶解的石墨烯，进一步制备成石墨烯/聚噻吩纳米复合材料，它可以有效提高聚噻吩的光电化学池光电转换效率，该光电开关比为 100，为太阳能转换、光电导、光检测器提供了一个可能。[[ljh-1116](#)]

17、由于石墨烯具有良好的机械、热学及电学性质，石墨烯-聚合物复合材料在分析化学各领域具有广阔应用前景。我们通过原位聚合的方法制备了新型聚乙二醇二甲基丙烯酸酯/石墨烯复合材料，并首次将其作为搅拌棒吸附萃取技术（SRSE）的萃取涂层，并应用于水样中萃取稠环芳烃类化合物。由于该石墨烯复合材料具有超高的比表面积，及与稠环芳烃类化合物之间的 π - π 相互作用，与不加石墨烯的聚合物相比，石墨烯-聚合物复合材料对水样中稠环芳烃类化合物具有更高的萃取效率。在最佳条件下，采用气质联用技术，建立了水样中稠环芳烃类化合物的 SRSE/GC-MS 分析方法，并成功地应用于实际水样的检测。以 3 倍信噪比来计算，16 种稠环芳烃类化合物的检测限在 0.005 到 0.429 ng mL^{-1} 之间，不同浓度的日内及日间精密度分别好于 12.5%和 12.6%。[[ljh-1117](#)]

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displayed an excellent sensitivity, together with a wide linear range and excellent stability for the detection of glucose. Accordingly, these unique properties of such novel nanocomposite generate a promising platform for the construction of mediator-free enzymatic biosensors. [[ljh-1106](#)]

7. A nanohybrid of gold nanoparticles (Au NPs) and chemically reduced graphene oxide nanosheets (cr-Gs) was synthesized by in situ growth of Au NPs on the surface of graphene nanosheets in the presence of poly(diallyldimethylammonium chloride) (PDDA), which not only improved the dispersion of Au NPs but also stabilized cholinesterase with high activity and loading efficiency. The obtained nanohybrid was characterized by TEM, XRD, XPS, and electrochemistry. Then an enzyme nanoassembly (AChE/Au NPs/cr-Gs) was prepared by self-assembling acetylcholinesterase (AChE) on Au NP/cr-Gs nanohybrid. An electrochemical sensor based on AChE/Au NPs/cr-Gs was further developed for ultrasensitive detection of organophosphate pesticide. The results demonstrate that the developed approach provides a promising strategy to improve the sensitivity and enzyme activity of electrochemical biosensors. [[ljh-1107](#)]

8. The self-assembly of tin dioxide (SnO_2) porous microspheres was conducted via a surfactant-free one step hydrothermal reaction. The crystalline structure and morphologies of the as-prepared samples were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The results show that the porous microspheres consist of single crystalline SnO_2 octahedral nanoparticles approximately 40 nm in width and 60 nm in length, with exposed high index {221} facets. The as-prepared porous nanostructure was used as an anode material for a lithium ion battery, whose cyclic voltammetry, electrochemical impedance, charge-discharge galvanstatic behavior and cycle performance were examined. A highly stable capacity about 690 mA g^{-1} after 50 cycles at a current density of 500 mA g^{-1} was achieved, which is much higher than that of nonassembled SnO_2 octahedral nanoparticles

应用高性能科学计算专用计算机集团，理论计算工作能够很好地进行。具体研究内容围绕着研究发展量子多体理论和计算方法；可以对原子、分子、团簇体系的物理性质和有关动力过程进行定量的理论计算和描述。具体如下：

1、我们仔细探讨了原子体系“准”完备基的概念和建立方法，提出一套可行的准完备建立方案。利用该方案可以对原子体系进行精密计算。具体的，我们对含有两个价电子的类 Mg 等电子系列进行了精密计算，定量阐明了由造成原子体系细节构分裂的 4 种机制（即自旋-轨道相互作用、电子交换作用的相对论校正、电子关联作用和 Breit 相互作用）间相互竞争所引起的 3snd 里德堡激发态精细结构的有趣变化；以及 $3s^2\ ^1S_0$, $3s3p\ ^1P_1$, $3s3p\ ^3P_{1,2}$ 之间的跃迁几率。[LJM-1101]

2、电子碰撞激发过程不论在量子多电子关联问题的基础研究方面而且在实际有关应用方面都具有重要意义。我们采用能够准确计算多电子原子的理论（R-矩阵理论），可以准确地计算电子与原子离子散射矩阵（S 矩阵）；根据 S 矩阵的解析性质，我们可以精确计算得到对应原子所有激发态能级。与精密实验光谱比较，通过理论计算能够清楚地阐明钠原子 $^2D_{5/2,3/2}$ Rydberg 系列反常精细结构。因此，充分证明理论计算的 S 矩阵 [$J^\pi=(5/s)^+$, $(3/2)^+$ 分量] 达到光谱的精度，同样地对其他 J^π 分量 [LJM-1102]。进而为获得精确的电子-离子碰撞截面提供一种方案；为相关重大科研项目（例如聚变能源研究、天体物理研究等）提供不可缺少的物理设计参数。

3、继续发展第一原理紧束缚态分子动力学理论以及相应的理论计算程序；它将可以计算较大的“团簇”而可以探索各种纳米结构的物理性质。利用“第一原理紧束缚态分子动力学理论计算程序”，我们探索碳球 C_{60} 是如何钻入单壁碳纳米管；尤其是当碳球 C_{60} 钻入临界单壁碳纳米管 (16,0) 时，由于该临界碳纳米管管口的驰豫而无法进入碳纳米管 [LJM-1103]。将对未来纳米科技应用有参考意义，例如纳米药学等。

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and irregular SnO_2 nanoparticles. The superior electrochemical properties result from the preferable nanostructure, with the pores favorable to the diffusion of electrolyte and providing buffer space for the volume change during alloying and dealloying reactions. Meanwhile, the special crystalline facets of the octahedral nanoparticles can facilitate Li^+ ion insertion and extraction. [ljh-1108]

9. Highly crystalline and thermally stable pure multi-walled $\text{Ni}_3\text{Si}_2\text{O}_5(\text{OH})_4$ nanotubes with a layered structure have been synthesized in water at a relatively low temperature of 200–210 °C using a facile and simple method. The nickel ions between the layers could be reduced *in situ* to form size-tunable Ni nanocrystals, which endowed these nanotubes with tunable magnetic properties. Additionally, when used as the anode material in a lithium ion battery, the layered structure of the $\text{Ni}_3\text{Si}_2\text{O}_5(\text{OH})_4$ nanotubes provided favorable transport kinetics for lithium ions and the discharge capacity reached 226.7 mA h g⁻¹ after 21 cycles at a rate of 20 mA g⁻¹. Furthermore, after the nanotubes were calcined (600 °C, 4 h) or reduced (180 °C, 10 h), the corresponding discharge capacities increased to 277.2 mA h g⁻¹ and 308.5 mA h g⁻¹, respectively. [ljh-1109]

10. Thermo-sensitive poly(N-isopropylacrylamide) hydrogel was used as a matrix polymer to immobilize polydiacetylenes (PDAs) vesicles. Blue-red chromic transition of PDAs was observed at lower temperature, compared to PDAs vesicle dispersion. The tuned chromic process was due to the interaction between matrix polymer and PDAs, especially the discontinuous volume phase transitions around the lower critical solution temperature of poly(N-isopropylacrylamide). [ljh-1110]

11. Hierarchical flower-like SnO_2 nanospheres have been prepared by one step hydrothermal reaction with surfactant-free. A possible growth mechanism is proposed. The application of this nanostructure in gas sensor for detecting ethanol reveals that the as-prepared SnO_2 nanospheres exhibit a high sensitivity and short response/recovery time. The flower-like SnO_2 nanostructures were also used as anode materials for Li-ion battery,

1、我们使用第一性原理方法研究了含拓扑线缺陷纳米带的电子性质。缺陷由碳原子的八边形以及两连接的五边形沿之字形方向作周期性重复得到。我们发现含这种线缺陷且边缘饱和的之字形石墨烯纳米带当线缺陷靠近某一边缘时会表现出半金属性。含线缺陷纳米带的电子性质可通过改变带的宽度以及线缺陷的位置来调节。当改变线缺陷的位置时，体系的电子性质会表现出由反铁磁半导体到反铁磁半金属再到铁磁金属的转变。由于这些丰富的电子与磁性质，含线缺陷之字形石墨烯纳米带在自旋电子学器件中可能具有潜在的应用。[NJ-1101-NJ-1103]

2、氢气是未来的清洁能源，如何才能安全有效的存储氢气是氢能利用的关键。储氢必须满足几个条件：（1）氢气的存储质量百分比要大于 6%；（2）氢气的吸附能要介于 0.2-0.6 eV 之间，如果氢气的吸附能太低，则氢气不容易被吸附住，如果氢气的吸附能太高，则氢气不利于释放；（3）吸附介质要能够稳定存在，不能由于氢气的吸附和释放而破坏吸附介质。我们研究发现，钙原子吸附在 BC₃ 平面上能够作为一种很好的储氢媒介。BC₃ 平面是目前实验上已经制备出来的一种二维平面，有类似于石墨烯的结构。钙原子能够稳定吸附在 BC₃ 平面上不会出现抱团。当一个钙原子吸附在 (2×2) BC₃ 平面上时，一个钙原子能够吸附六个氢气分子，每一个氢气分子的吸附能都在 0.2-0.6 eV 之间。为了提高氢气的存储量，我们采用钙原子双面吸附的方式，在 (1×1) 的 BC₃ 原胞中，上下两面分别吸附一个钙原子。钙原子双面吸附之后发现，钙原子的最近邻距离大于钙的体结构中钙原子的最近邻距离，钙的吸附能大于钙的体结构的结合能。进一步，我们采用第一原理分子动力学验证了吸附结构的稳定性。当双面吸附钙原子后，每一个钙原子能够吸附四个氢气分子，储氢质量百分比高达 8.4%，氢气分子的平均吸附能是 0.28 eV。计算表明，钙吸附后的 BC₃ 平面能够作为一种高效的储氢材料。[NJ-1104-NJ-1106]

我们通过第一性原理计算的方法研究了碱金属或碱土金属铁基砷化物 Ax(FeAs)_{1-x} 的稳定结构。我们发现 (1) 组分 x=1/3 的所有“122”类型的已知的实验结构都是稳定的；(2) 组分 x=1/2 的所有“111”类型的结构除了

whose cyclic voltammetry, charge-discharge galvanostatic behavior and cycle performance were examined. For the sample with 6 h hydrothermal time, a highly stable capacity about 570 mAh_g⁻¹ after 100 cycles is achieved. The gas sensing properties are mainly determined by the specific surface area, and the 3D nanostructured films composed of flower-like SnO₂ nanospheres are favorable for the diffusion of gas molecules. At the same time, the high specific surface area of the flower-like SnO₂ nanospheres can provide more electrochemical active sites for Li storage, and the 3D nanostructured films composed of this nanostructure facilitate the diffusion of electrolyte. Furthermore, the short rods on the nanospheres may provide a buffer to alleviate volume change during the alloying and dealloying reactions between Sn and Li. The superior properties achieved here suggest that the as-prepared hierarchical flower-like SnO₂ nanostructures have potential application in Li-ion battery and gas sensor. [ljh-1111]

12. Sensitive and selective detection of DNA is in urgent need due to its important role in human bodies. Many disorders, such as Alzheimer's disease and various cancers, are closely related with DNA damage. In this work, a novel electrochemical DNA biosensor was constructed on a DNA-assembling graphene platform which provided a robust, simple and biocompatible platform with large surface area for DNA immobilization. The as-designed DNA sensor was fabricated by directly assembling captured ssDNA on a graphene-modified electrode through the p-p stacking interaction between graphene and ssDNA bases. Then, the target DNA sequence and oligonucleotide probes-labeled AuNPs were able to hybridize in a sandwich assay format, following the AuNPs-catalyzed silver deposition. The deposited silver was further detected by differential pulse voltammetry. Owing to the high DNA loading ability of graphene and the distinct signal amplification by AuNPs-catalyzed silver staining, the resulting biosensor exhibited a good analytical performance with a wide detection linear range from 200 pM to 500 nM, and a low detection limit of 72 pM. Additionally, the biosensor was proved to be able to

CsFeAs 之外都是稳定的; (3)除了 1/3 和 1/2 组分, 组分为 $x=3/4$ 的 K_3FeAs 是稳定的。预测的稳定结构 $KFeAs$, $RbFeAs$, $SrFeAs$, $BaFeAs$, K_3FeAs 的 As-Fe-As 键角接近理想四面体键角, 表明它们可能为超导体。我们还研究了稳定结构的磁有序基态。[[NJ-1107](#)]

我们通过第一性原理的方法研究了 3d 过渡金属锑化物 $A_x(TMSb)_{1-x}$ 的结构性质。我们发现稳定化合物集中在 $x=1/3$ 和 $1/2$ 组分, 分别对应于“122”和“111”类型的体系。对于钙基系统, $CaNi_2Sb_2$ 和 $CaTMSb$ 是稳定的。对于锶基系统, $SrTM_2Sb_2$ 和 $SrTMSb$ 是稳定的。对于钡基系统, $BaTM_2Sb_2$ 和 $BaTMSb$ 是稳定的。随着过渡金属 3d 电子的增加, $SrTM_2Sb_2$ 和 $BaTM_2Sb_2$ 都显示出从 $ThCr_2Si_2$ 类型结构到 $CaBe_2Ge_2$ 类型结构的转变。这个转变与结构参数 TMSb 键长有关, 表现为层内和层间 TMSb 键相互作用的竞争。我们也研究了稳定结构的磁有序基态。[[NJ-1108](#)]

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研究了经典信息删除和量子信息删除的区别 [[lgl-1101](#)], 给出了高维电子纠缠态的纯化方案 [[lgl-1102](#)], 高维体系的量子纠缠的刻画 [[lgl-1103](#)]。撰写了一篇有关对偶量子计算的综述论文 [[lgl-1104](#)]。在实验上实现了一个量子定点算法 [[lgl-1105](#)]。给出了高维体系的傅里叶变换量子算法 [[lgl-1106](#)]。我们给出了对偶量子计算中零波函数的佯谬解释 [[lgl-1107](#)]。提出了一种基于 Grover 算法的量子秘密共享方案, 并在 NMR 体系中进行了实验演示 [[lgl-1108](#)]。给出了量子搜索算法的分解几何解释 [[lgl-1109](#)]。在理论上给出了任意量子体系的无消相干子空间 [[lgl-1110](#)], 给出了量子门的任意子实现方案 [[lgl-1111](#)]。

grown directly on transparent conductive glass (FTO) were prepared by a facile two-step wet chemical synthesis process, using a simple aqueous chemical growth method involving immersing the TiO_2 nanorod arrays in an aqueous $TiCl_4$ solution as seeds, which were prepared by a hydrothermal method. The dye-sensitized solar cells based on the TiO_2 nano-branched arrays which were only about 3 mm in length show a short-circuit current intensity of 10.05 mA cm^{-2} and a light-to-electricity conversion efficiency of 3.75%, which is nearly three times as high as that of bare nanorod arrays, due to the preferable nanostructure, which not only retains the efficient charge separation and transport properties of the nanorod arrays, but also can improve the amount of dye adsorption due to the increased specific surface area from the nanobranches. [[lgh-1114](#)]

discriminate the complementary sequence from the single-base mismatch sequence. The simple biosensor is promising in developing electronic, on-chip assays in clinical diagnosis, environmental control, and drug discovery. [[lgh-1112](#)]

13. In this Application Note, we describe, for the first time, the rapid analysis of hydrophobic compounds present in environmental contaminants, which includes polycyclic aromatic hydrocarbons (PAHs) and estrogen, by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF MS) with the use of graphene as matrix. MALDI-TOF MS with conventional matrix has limitations in analyzing low-polarity compounds owing to their difficulty in ionization. We demonstrate that compared with conventional matrix, graphene displays higher desorption/ionization efficiencies for PAHs, and no fragment ions are observed. The method also holds potential in quantitative analysis. In addition, the ionization signal increases with the increasing number of benzene rings in the PAHs, suggesting that graphene binds to PAHs via π - π stacking interactions. Furthermore, graphene as adsorbent for solid-phase extraction of coronene from river water sample displays good performance with a detection limit of 10⁻⁷ M. This work provides a novel and convenient method for analyzing low-polarity environmental contaminants by MALDI-TOF MS. [[lgh-1113](#)]

14. Hierarchical TiO_2 nanostructures would be desirable for preparing dye-sensitized solar cells because of their large amount of dye adsorption and superior light harvesting efficiency, as well as efficient charge separation and transport properties. In this study, rutile TiO_2 nano-branched arrays

15. Electrochemical DNA sensors have been increasingly fascinating due to high sensitivity, specificity, portability and integrated compatibilities with microelectronics. Numerous strategies have been developed to design electrochemical DNA sensors with high sensitivity and selectivity. In this review, we will focus on the efforts toward sensitive electrochemical DNA sensing based on nanomaterials including metal nanoparticles, magnetic nanoparticles, semiconductor nanoparticles and carbon nanomaterials, especially carbon nanotubes. The potential application of the electrochemical DNA sensors in gene analysis, diagnosis, environmental and food safety monitoring will be briefly discussed. At the end of this review, we will give a brief outlook of the future challenges of electrochemical DNA sensors. [[ljh-1115](#)]

16. A novel photoelectrochemical cell (PEC) based on graphene/P3OT (poly(3-octyl-thiophene)) nanocomposites was developed for photovoltaic solar energy conversion. Based on the noncovalent functionalization with pyrenebutyrate (PB), solution processable graphene was achieved and used to prepare the graphene/P3OT nanocomposites for PEC application. It has been shown that the doping of the graphene in P3OT film significantly improved the photocurrent as well as the photovoltaic conversion efficiency of the PEC cells by over 10 folds. The highest on-off ratio of photocurrent from the graphene/P3OT nanocomposites reached about 100. Moreover, the performances of the photoelectrochemical cells were largely dependent on the graphene content and morphology of the graphene/P3OT nanocomposites, and the highest photovoltaic conversion efficiency was obtained at a graphene content of 5 wt.% in the nanocomposites. The solution-processed graphene/P3OT nanocomposites PEC provides a general platform for next generation solar energy conversion, photoconductivity and photodetectors. [[ljh-1116](#)]

17. Due to the excellent mechanical, thermal and electrical properties, graphene/polymer composite is expected to have a variety of applications in analytical chemistry. In this study, a new poly(ethylene glycol dimethacrylate)/graphene composite was prepared by in situ polymerization. The new composite was used for the first time as the extraction coating of stir rod sorptive extraction for the preconcentration of polycyclic aromatic hydrocarbons (PAHs) from water samples. Because of the high specific surface area and p-p electrostatic stacking properties of graphene, the graphene-polymer composite showed higher extraction efficiencies towards most target PAHs from water samples than the neat polymer. Under the optimal conditions, a method for the determination of PAHs in water samples was proposed based on the combination of stir rod sorptive extraction (SRSE) and gas chromatography-mass spectrometry (GC-MS). The limit of detection (LODs) of the developed method for 16 PAHs ranged from 0.005 to 0.429 ng mL⁻¹, depending on the compound. Good reproducibility of method was obtained as intra- and inter-day precisions, the relative standard deviations (RSDs) were less than 12.5% and 12.6%, respectively. Due to the excellent mechanical, thermal and electrical properties, graphene/polymer composite is expected to have a variety of applications in analytical chemistry. In this study, a new poly(ethylene glycol dimethacrylate)/graphene composite was prepared by in situ polymerization. The new composite was used for the first time as the extraction coating of stir rod sorptive extraction for the preconcentration of polycyclic aromatic hydrocarbons (PAHs) from water samples. Because of the high specific surface area and p-p electrostatic stacking properties of graphene, the graphene-polymer composite showed higher extraction efficiencies towards most target PAHs from water samples than the neat polymer. Under the optimal conditions, a method for the determination of PAHs in water samples was proposed based on the combination of stir rod sorptive extraction (SRSE) and gas chromatography-mass spectrometry (GC-MS). The limit of detection (LODs) of the developed method for 16 PAHs ranged from 0.005 to 0.429 ng mL⁻¹, depending on the compound. Good reproducibility of method was obtained as intra- and inter-day precisions, the relative standard deviations (RSDs) were less than 12.5% and 12.6%, respectively. [[ljh-1117](#)]

Theoretical Division

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With the high-performance specialized parallel PC cluster, our theoretical computations have been carried out. Our research centers around developments of many-body quantum theories and computation methods; More specifically we carry out theoretical calculations of properties and related dynamical processes for atomic, molecular and cluster systems. More specifically as follows:

1. We have proposed a workable scheme to construct the "quasi-complete basis" for general atomic systems. Using such scheme we can perform precision calculations in atomic systems. More specifically, we have carried out calculations in Mg-like isoelectronic sequences with two valance electrons. We have elucidated the four competing mechanisms(i.e., spin-orbit interactions, relativistic corrections of electron exchange interactions, electron correlations, and Breit interactions) of fine structures splitting variations in 3rd Rydberg series clearly; and also calculated the radiative transition rates among $3s^2\ ^1S_0$, $3s3p\ ^1P_1$, $3s3p\ ^3P_{1,2}$ states. [[LJM-1101](#)]

2. Electron-impact excitation processes are of fundamental and practical importance. Adopt the R-matrix method which can treat precisely all important atomic energy states, we can accurately calculate the scattering matrix (S matrix) for electron-ion collisions. Through the analytical property of S matrix, we can calculate the energy levels of all excited states for the corresponding atoms. By comparing with the accurate spectroscopic data, our theoretical calculation results are accurate enough to elucidate the anomalous fine structures of $^2D_{5/2,3/2}$ Rydberg series for Na atoms. It indicates that our calculated S matrix for the $J^\pi=(5/2)^+, (3/2)^+$ components have reached the spectroscopic precisions, similarly for the other J^π components. [[LJM-1102](#)]

Therefore, it provides a scenario to obtain cross sections of electron-ion collisions with spectroscopic accuracy which should be very useful in various application fields such as fusion researches, researches in astrophysics etc.

3. We continue to develop a first-principle tight-binding molecular dynamics computation code in order to calculate cluster systems with a relatively large number of atoms or molecules which will provide various informations about various "nano structures". We adopt the tight-binding molecular dynamics method to study encapsulation processes C_{60} into single carbon nanotubes. for a (16,0) nanotube, it is impossible to encapsulate C_{60} into the tube because of a much larger energy barrier with the relaxation of the open end of the tube. [[LJM-1103](#)] Such studies may be useful for potential applications in pharmaceutical molecule encapsulation processes.

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1. First-principles calculations have been performed to investigate the electronic properties of graphene nanoribbons with topological line defects composed of octagons and fused pentagons. We find that the edge-passivated zigzag graphene nanoribbons (ZGNRs) with the line defects along the edge show half-metallicity as the line defect is close to one edge. The electronic properties of the ZGNRs with line defects can be tuned by changing the ribbon width and the position of the line defect. When the position of the line defect changes, there are transitions from an antiferromagnetic semiconductor to an antiferromagnetic half-metal, and then to a ferromagnetic metal, suggesting the potential applications of the system in spintronic devices. [[NJ-1101-NJ-1103](#)]

2. Hydrogen has been recognized as an ideal energy resource for future energy schemes because of its efficiency, abundance and environmental friendliness. The safe storage is important for its wide application as the future fuel. The hydrogen storage material should meet the requirements of high gravimetric/volumetric density, fast kinetics, favorable thermodynamics and good reversibility. The BC_3 sheet has been produced experimentally. We expect that BC_3 sheet could be used as an efficient hydrogen storage medium. We study the hydrogen storage on the calcium-decorated BC_3 sheet by first principles calculations, and find that the Ca atoms can be strongly adsorbed on BC_3 sheet

without clustering, which facilitates the reversible hydrogen adsorption and desorption. For one Ca atom adsorbing on the (2×2) BC₃ unit cell, each Ca could adsorb up to six hydrogen molecules. By adsorbing Ca atoms on both sides of BC₃ sheet to form (1×1) pattern, a hydrogen capacity up to 8.4 wt% can be achieved and the average binding energy of hydrogen molecules adsorbed by Ca atoms is about 0.28 eV. [[NJ-1104-NJ-1106](#)]

3. We have investigated the structural stabilities of iron arsenide compounds A_x(FeAs)_{1-x} (A=alkali and alkaline-earth metals) by first principles calculations. We find that (i)all of the experimental “122” type structures with composition x=1/3 are stable; (ii)all of the “111” type structures with composition x=1/2 except CsFeAs are stable; (iii)K₃FeAs with composition x=3/4 is stable. The predicted stable KFeAs, RbFeAs, SrFeAs, BaFeAs, K₃FeAs have the As-Fe-As bond angles close to the ideal tetrahedral angles, indicating that they may be superconductors. [[NJ-1107](#)]

4. We have investigated the structural properties of 3d transition metal antimonide compounds A_x(TMSb)_{1-x} by first principles calculations. We find that the stable compounds focus on x=1/3 and 1/2 compositions, correspond to the “122” and “111” type systems, respectively. For Ca-system, CaNi₂Sb₂ and CaTMSb are stable. For Sr-system, SrTM₂Sb₂ and SrTMSb are stable. For Ba-system, BaTM₂Sb₂ and BaTMSb are stable. SrTM₂Sb₂ and BaTM₂Sb₂ show the transition from the ThCr₂Si₂-type structure to the CaBe₂Ge₂-type structure with the increasing transition metal 3d electrons. The transition is in connection with the intralayer and interlayer TMSb bond length in the CaBe₂Ge₂-type structure. The stable compounds have various magnetic ground states. [[NJ-1108](#)]

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We studied the difference between classical deletion and quantum deletion [[gll-1101](#)], proposed an entanglement purification protocol for high dimension electronic state [[gll-1102](#)], a measure for multipartite quantum entanglement [[gll-1103](#)]. We wrote a review article about duality quantum computing [[gll-1104](#)]. Experimentally, we demonstrated a quantum fixed-point search algorithm [[gll-1105](#)]. We gave the Fourier transform for high dimension system [[gll-1106](#)]. We gave a solution to the zero-wave function paradox in duality quantum computer.[[gll-1107](#)] We proposed a quantum secret sharing protocol based on Grover algorithm and experimentally demonstrated the protocol. [[gll-1108](#)] We gave a geometric explanation of the quantum search algorithm. [[gll-1109](#)] We theoretically studied the decoherence free subspace for anyon quantum systems [[gll-1110](#)], and the quantum gate in using anyons. [[gll-1111](#)]

论文清单 (Publication List)

《总共 82 篇; 其中 (★) 为 SCI 论文, 共 75 篇 SCI 论文》

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章程

一、《原子分子纳米科学研究中心》(以下简称《中心》)设立四个研究部。

二、《中心》长期追求的科学目标是围绕着原子、分子层次的超灵敏探测、超灵敏识别、操纵和控制。《中心》将以全方位的方式向国内、外教育与科研界开放。欢迎国内外有志于从事这方面研究的科学家参加《中心》的科研工作。

三、《中心》设立管理委员会,学术委员会。日常工作由《中心》主任负责,副主任分工协助主任工作,重大问题由主任主持的主任会议讨论。《中心》教授有权对《中心》发展过程中的一些重要问题所提出的咨询意见和建议。

四、《中心》学术委员会主任、副主任以及《中心》主任、副主任由清华大学聘任。《中心》学术委员会委员由《中心》聘任。《中心》实验室主任、副主任和理论部主任由《中心》聘任。《中心》成员和客座成员由《中心》聘任。

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1. The Center for Atomic and Molecular Nanosciences consists of four research divisions.

2. Research of the Center covers the following areas: ultrasensitive detection, ultrasensitive recognition, manipulation and control of atoms and/or molecules. The Center of Atomic and Molecular Nanosciences welcomes both domestic and foreign colleagues with common interests to join us to carry out cooperative researches.

3. There are two special Committees; Supervisory Committee and Scientific Committee. The Director of the Center of Atomic and Molecular Nanosciences is in charge of the Center. The decision of vitally important issues will be determined at the Director Meeting chaired by the Director. The members of the Center have right to make their suggestions concerning the Center.

4. The Chairman and the Deputy Chairmen of the Scientific Committee as well as the Director and Deputy Directors of the Center of Atomic and Molecular Nanosciences are appointed by Tsinghua University. The Members of the Scientific Committee are appointed by the Center of Atomic and Molecular Nanosciences. The Directors and Co-directors of the research divisions as well as the members (including visiting members) of the Center are appointed by the Center.

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