Jeffrey Reimers, Wei Ren
Department of Physics,
International Center for Quantum and Molecular Structures,
Shanghai University, Shanghai 200444, China

杰夫 任伟

上海大学理学院物理系
上海大学量子与分子结构国际中心

三、服务国家战略

习近平总书记2014年明确要求：上海建成具有全球影响力的科技创新中心

量子科学技术成为中国实现伟大复兴的驱动力，是国家战略的重中之重

2014年任伟主持成立——上海大学量子与分子结构国际中心

International Centre for Quantum and Molecular Structures

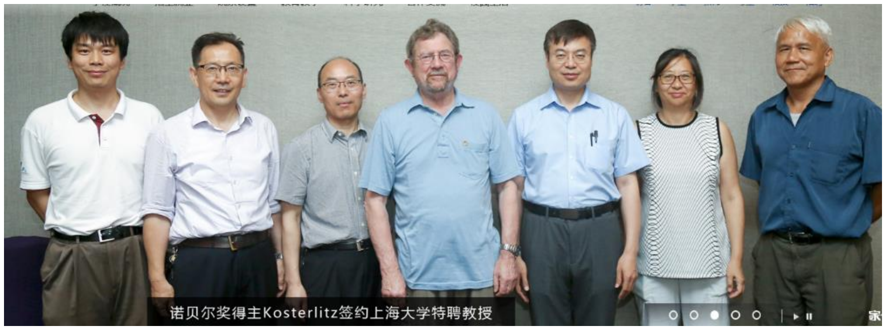
同时支撑建设

上海市高温超导重点实验室和**上海大学材料基因组工程研究院**

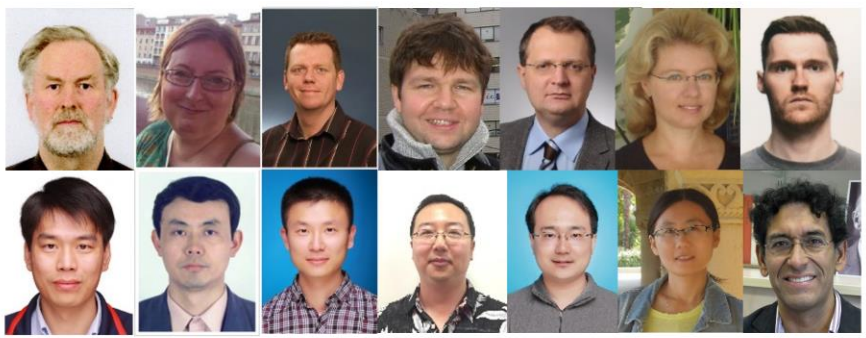
省部共建高品质特殊钢冶金与制备国家重点实验室

三、服务国家战略

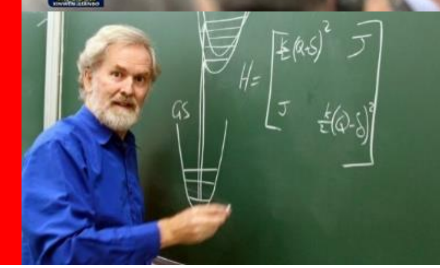
引进拓扑物理诺贝尔奖得主J.M. Kosterlitz



澳、波、美、俄、西、英7位非华裔全职教授



习近平主席2014年
李克强总理2016年
接见上海大学全职教授
澳大利亚科学院院士
杰夫Jeffrey Reimers
为上海市政协谏言
中国日报、Nature专访



上海大学量子与分子结构国际中心近五年在量子物理和化学科学等领域取得了世界一流的研究成果，在包括Science 、Nature、Nature Chemistry、 Nature Reviews Chemistry、PNAS、 PRL、JACS等期刊发表了200多篇论文。

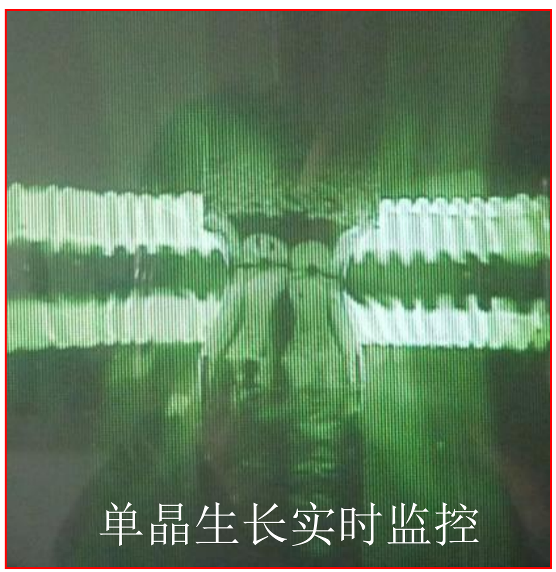
三、服务国家战略

1. 2019/7/1-7 国际晶体学会计算晶体学和拓扑绝缘体暑期学校
2. 2018/11/18-23 密度泛函理论Exciting计算和材料数据国际研讨会
3. 2018/9/24-26 第14届新加坡/中国物理学前沿研讨会
4. 2017/6/11-17 国际晶体学会上海计算晶体研讨会
5. 2017/1/16-17 鸿之微、麦吉尔大学郭鸿RESCU软件发布会暨培训会议
6. 2016/10/7-10 第8届APCTP多铁性材料国际研讨会
7. 2016/6/22-26 第9届计算纳米科学与新能源材料国际研讨会
8. 2016/5/28-29 第275期东方科技论坛-集成电路中的新兴电子材料和器件
9. 2015/12/11-12 第268期东方论坛-未来集成电路中的新兴电子材料和器件
10. 2015/11/25 先进材料中的光电磁学现象专题学术研讨会
11. 2015/1/21-23 上海大学光合作用低能量激发态国际研讨会
12. 2014/6/10-13 新兴电子材料和器件物理EEMD国际研讨会【鸿之微成立】

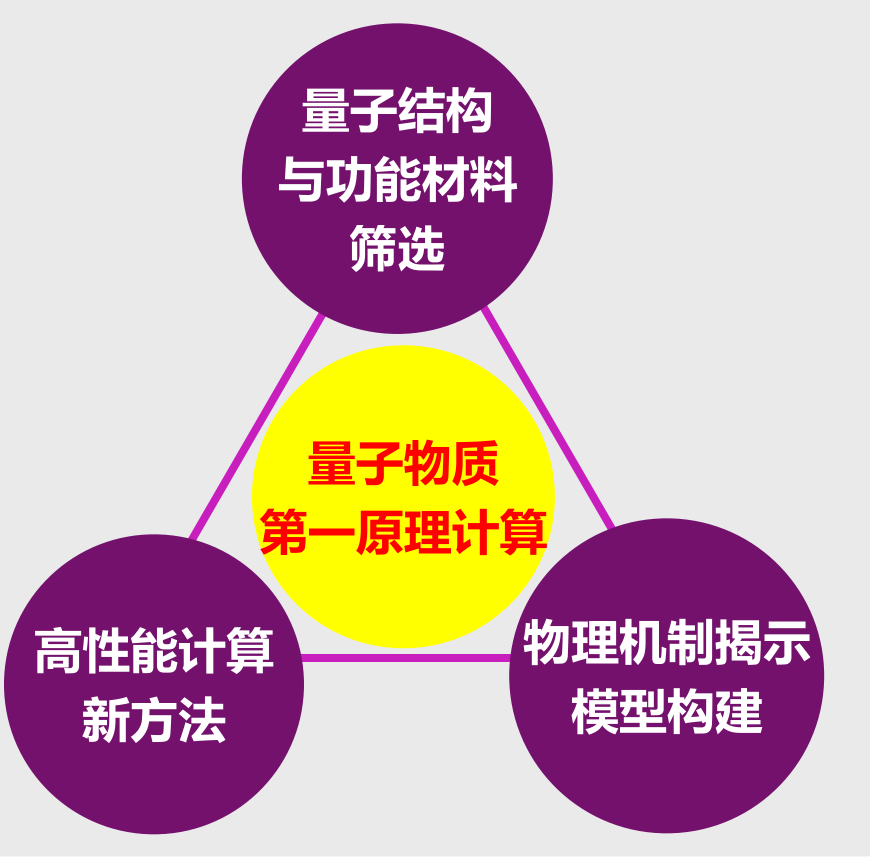
四、工作发展潜力

上海大学自强4000、上海超算中心、无锡神威太湖之光、广州天河二号

候选人的高性能计算实验室也经过四期建设，初步建成3000个CPU核心、100个GPU的强大服务器集群用于量子力学第一原理计算科学研究。



四、工作发展潜力



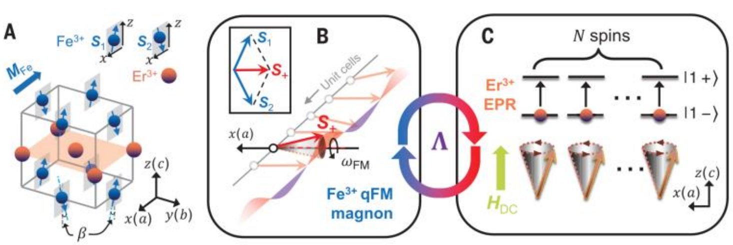
- 揭示量子材料器件关联电子自旋轨道耦合磁电耦合机制；
- 理论计算与实验相结合探索二维体系和钙钛矿结构应用；
- 发展磁性/铁电多铁材料关键单晶合成制备设计表征技术。

总体目标：发展新兴量子材料和器件的计算和设计

上海大学理学院物理系2018年在Science上发表论文

上海大学曹世勋、马国宏、任伟教授团队在量子磁性体系中首次观测了量子光学中Dicke协同作用的实例。该研究成果以 “Observation of Dicke Cooperativity in Magnetic Interactions”为题在国际著名顶级期刊Science发表。

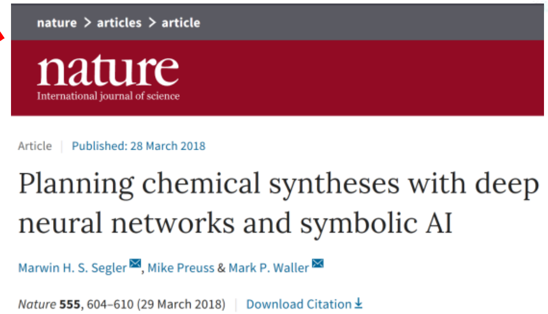
创新团队曹世勋教授为通讯作者，东方学者跟踪计划任伟教授、东方学者马国宏教授、青年东方学者金钻明博士、硕士研究生袁宁、向茂林、徐凯等同学为共同作者。本工作得到了上海市教委和科委、国家自然科学基金、国家科技部的资助。



Mark Waller教授2018年人工智能领域Nature论文

上海大学量子与分子结构国际中心
上海大学理学院物理系东方学者

Altmetric = 552
Citations = 74


nature > articles > article

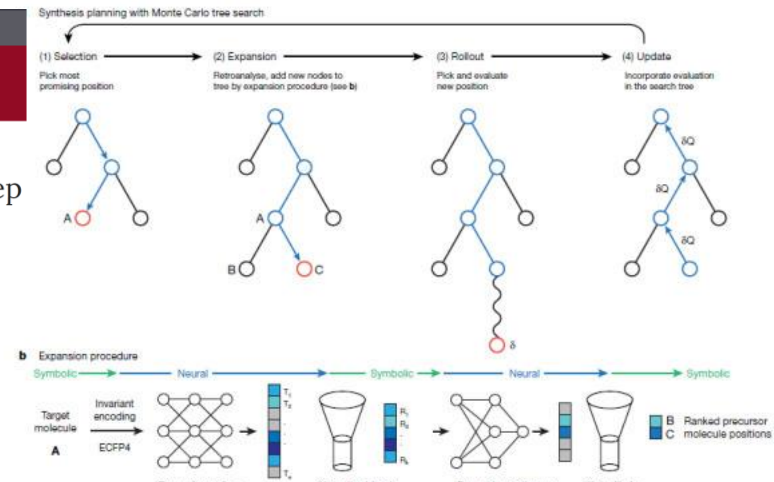
nature
International journal of science

Article | Published: 28 March 2018

Planning chemical syntheses with deep neural networks and symbolic AI

Marwin H. S. Segler, Mike Preuss & Mark P. Waller

Nature **555**, 604–610 (29 March 2018) | Download Citation



“ Planning chemical syntheses with deep neural networks and symbolic AI” 是Mark Waller教授2016年3月全职加入上大以后，设计指导整个项目并发表的一篇具有重大国际影响力的人工智能领域学术论文。

开发蒙特卡洛树进行搜索，并引入符号人工智能来寻找逆合成分析的路线。并在蒙特卡洛树步骤还中引入了两种深度神经网络来提高计算精度与效率：扩张决策网络用于寻找路径，过滤网络用于对可能的逆合成路线进行初步筛选。用于训练神经网络的测试集包括了所有已经发表过的有机化学反应。Mark Waller教授开发出的分析系统比传统的计算机辅助法快30倍，预测出的合成路线比传统计算机辅助法给出的多一倍，堪称化学领域的阿尔法狗。

上海大学理学院物理系全职教授、量子与分子结构国际中心(ICQMS)主任、澳大利亚科学院院士 Jeffrey Reimers教授与悉尼大学、澳大利亚国立大学的合作者提出

上海大学为论文

Maxwell Cross

Jeffrey Reimer

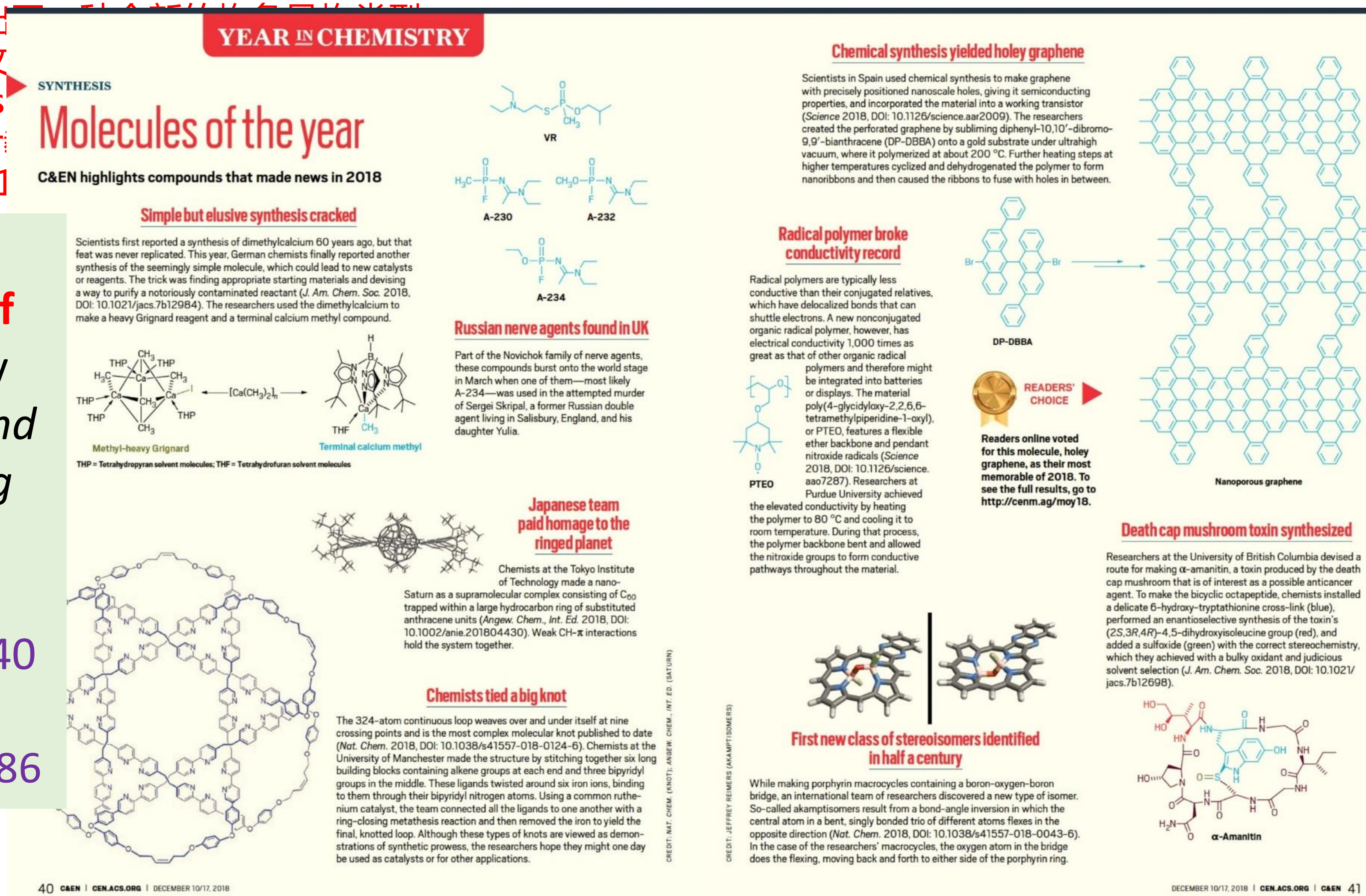
继在PNAS (201

Voted **#2 molecule of the year** by *Chemistry and Engineering News*

150,000 readers in 140 countries

Altmetric = 186

式的重要发现。



YEAR IN CHEMISTRY

SYNTHESIS

Molecules of the year

C&EN highlights compounds that made news in 2018

Simple but elusive synthesis cracked

Scientists first reported a synthesis of dimethylcalcium 60 years ago, but that feat was never replicated. This year, German chemists finally reported another synthesis of the seemingly simple molecule, which could lead to new catalysts or reagents. The trick was finding appropriate starting materials and devising a way to purify a notoriously contaminated reactant (*J. Am. Chem. Soc.* 2018, DOI: 10.1021/jacs.7b12984). The researchers used the dimethylcalcium to make a heavy Grignard reagent and a terminal calcium methyl compound.

Methyl-heavy Grignard ← $[Ca(CH_3)_2]_n$ → Terminal calcium methyl

THP = Tetrahydropyran solvent molecules; THF = Tetrahydrofuran solvent molecules

VR A-230 A-232 A-234

Russian nerve agents found in UK

Part of the Novichok family of nerve agents, these compounds burst onto the world stage in March when one of them—most likely A-234—was used in the attempted murder of Sergei Skripal, a former Russian double agent living in Salisbury, England, and his daughter Yulia.

Japanese team paid homage to the ringed planet

Chemists at the Tokyo Institute of Technology made a nano-Saturn as a supramolecular complex consisting of C_{60} trapped within a large hydrocarbon ring of substituted anthracene units (*Angew. Chem., Int. Ed.* 2018, DOI: 10.1002/anie.201804430). Weak CH-π interactions hold the system together.

Chemists tied a big knot

The 324-atom continuous loop weaves over and under itself at nine crossing points and is the most complex molecular knot published to date (*Nat. Chem.* 2018, DOI: 10.1038/s41557-018-0124-6). Chemists at the University of Manchester made the structure by stitching together six long building blocks containing alkene groups at each end and three bipyridyl groups in the middle. These ligands twisted around six iron ions, binding to them through their bipyridyl nitrogen atoms. Using a common ruthenium catalyst, the team connected all the ligands to one another with a ring-closing metathesis reaction and then removed the iron to yield the final, knotted loop. Although these types of knots are viewed as demonstrations of synthetic prowess, the researchers hope they might one day be used as catalysts or for other applications.

CREDIT: NAT. CHEM. (KNOT); ANGEW. CHEM., INT. ED. (SATURN)

40 C&EN | CEN.ACS.ORG | DECEMBER 10/17, 2018

Chemical synthesis yielded holey graphene

Scientists in Spain used chemical synthesis to make graphene with precisely positioned nanoscale holes, giving it semiconducting properties, and incorporated the material into a working transistor (*Science* 2018, DOI: 10.1126/science.aar2009). The researchers created the perforated graphene by subliming diphenyl-10,10′-dibromo-9,9′-bianthracene (DP-DBBA) onto a gold substrate under ultrahigh vacuum, where it polymerized at about 200 °C. Further heating steps at higher temperatures cyclized and dehydrogenated the polymer to form nanoribbons and then caused the ribbons to fuse with holes in between.

DP-DBBA → Nanoporous graphene

Radical polymer broke conductivity record

Radical polymers are typically less conductive than their conjugated relatives, which have delocalized bonds that can shuttle electrons. A new nonconjugated organic radical polymer, however, has electrical conductivity 1,000 times as great as that of other organic radical polymers and therefore might be integrated into batteries or displays. The material poly(4-glycidyloxy-2,2,6,6-tetramethylpiperidine-1-oxyl), or PTEO, features a flexible ether backbone and pendant nitroxide radicals (*Science* 2018, DOI: 10.1126/science.aao7287). Researchers at Purdue University achieved the elevated conductivity by heating the polymer to 80 °C and cooling it to room temperature. During that process, the polymer backbone bent and allowed the nitroxide groups to form conductive pathways throughout the material.

PTEO

READERS' CHOICE

Readers online voted for this molecule, holey graphene, as their most memorable of 2018. To see the full results, go to http://cenm.ag/moy18.

Death cap mushroom toxin synthesized

Researchers at the University of British Columbia devised a route for making α-amanitin, a toxin produced by the death cap mushroom that is of interest as a possible anticancer agent. To make the bicyclic octapeptide, chemists installed a delicate 6-hydroxy-tryptathionine cross-link (blue), performed an enantioselective synthesis of the toxin's (2*S*,3*R*,4*R*)-4,5-dihydroxyisoleucine group (red), and added a sulfoxide (green) with the correct stereochemistry, which they achieved with a bulky oxidant and judicious solvent selection (*J. Am. Chem. Soc.* 2018, DOI: 10.1021/jacs.7b12698).

α-Amanitin

First new class of stereoisomers identified in half a century

While making porphyrin macrocycles containing a boron-oxygen-boron bridge, an international team of researchers discovered a new type of isomer. So-called akamptisomers result from a bond-angle inversion in which the central atom in a bent, singly bonded trio of different atoms flexes in the opposite direction (*Nat. Chem.* 2018, DOI: 10.1038/s41557-018-0043-6). In the case of the researchers' macrocycles, the oxygen atom in the bridge does the flexing, moving back and forth to either side of the porphyrin ring.

CREDIT: JEFFREY REIMERS (AKAMPTISOMERS)

DECEMBER 10/17, 2018 | CEN.ACS.ORG | C&EN 41

Faraday cage screening reveals intrinsic aspects of the van der Waals attraction

Musen Li (李木森)[a,b], ...frey R. Reimers[a,b,c,1], John F. Dobson[d,e], and Tim Gould[d,e,1]

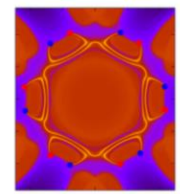
...ternational Centre f... ...antum and Molecular Structures, Shanghai University, Shanghai 200444, China; [b]Department of Physics, Shanghai University, ... School of Mathematical and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia; [d]School of Natural Scienc... ...niversity, Nathan, QLD 4111, Australia; and [e]Queensland Micro- and Nanotechnology Centre, Griffith University, Nathan, QLD 4111, Australia

Edited by John P. Perdew, Temple University, Philadelphia, PA, and approved September 21, 2018 (received for review July 5, 2018)

First papers with SHU first-author students in these two journals

上海大学量子与分子结构国际中心
理学院物理系博士生
李木森发表一作PNAS
高恒发表一作PRL

PRL编辑推荐



Dirac-Weyl semimetal: Coexistence of Dirac and Weyl fermions in polar hexagonal ABC crystals

Heng Gao *et al.*
Phys. Rev. Lett. **121**, 106404 (2018)

Published 5 September 2018

PHYSICAL REVIEW LETTERS **121,** 106404 (2018)

Editors' Suggestion

Dirac-Weyl Semimetal: Coexistence of Dirac and Weyl Fermions in Polar Hexagonal ABC Crystals

Heng Gao,[1,2] You... ...uk Kim,[2,3] Jörn W. F. Venderbos,[2,4] C. L. Kane,[4] E. J. Mele,[4] Andrew M. Rappe,[2,*] and Wei Ren[1,†]

...nternational Centre for Quantum and Molecular Structures, Materials Genome Institute,
Shanghai K... ...ratory of High Temperature Superconductors, Physics Department, Shanghai University, Shanghai 200444, China
...Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA
[3]Department of Physics, Sungkyunkwan University, Suwon 440-746, Korea
[4]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6396, USA

(Received 13 February 2018; published 5 September 2018)

has been highlighted by the editors as an Editors' Suggestion. Publication of a Letter is already a considerable achievement, as *Physical Review Letters* accepts fewer than 1/4 of submissions, and is ranked first among physics and mathematics journals by the Google Scholar five-year h-index. A highlighted Letter has additional significance, because only about one Letter in six is highlighted as a Suggestion due to its particular importance, innovation, and broad appeal. Suggestions are downloaded twice as often as the average Letter, and are covered in the press substantially more often. If Suggestions were a separate publication, they would have an Impact Factor of 17. More information about our journal and its history can be found on our webpage prl.aps.org.

Yours sincerely,

Hugues Chaté
Editor
Physical Review Letters

Michael Thoennessen
Editor in Chief
Physical Review

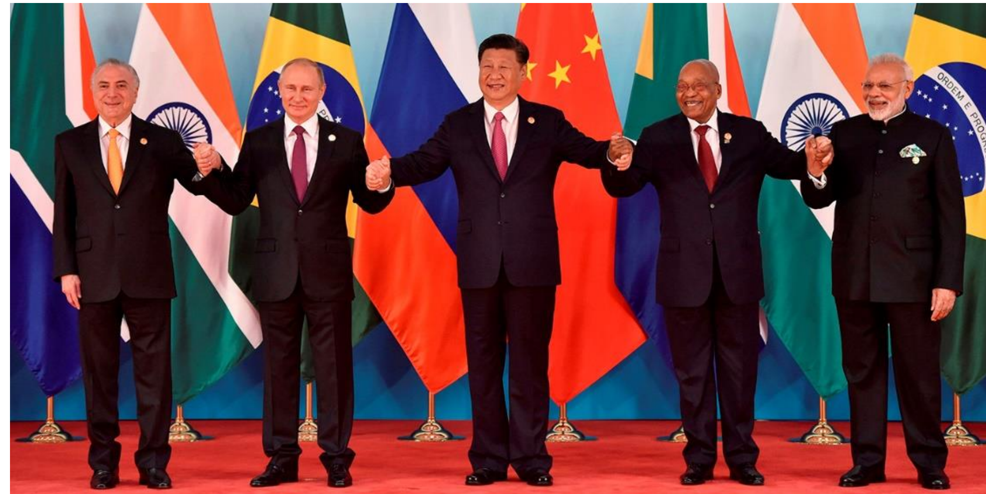
Wei Ren 2018 NSFC key grant

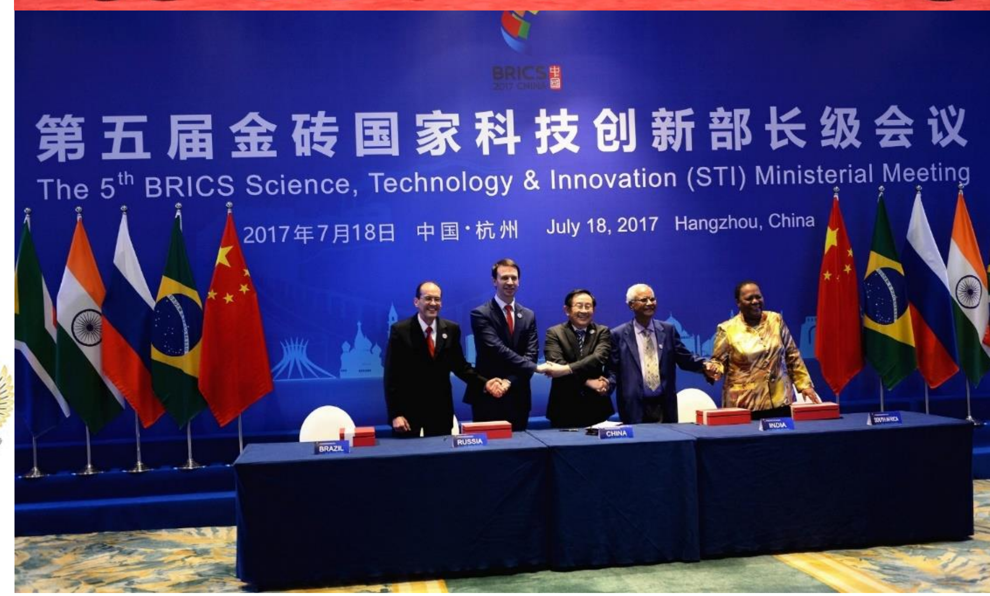
任伟2018年国际重点基金

国家自然科学基金委员会与金砖国家科技创新框架计划合作研究项目

项目批准号：51861145315
项目名称：多铁性材料的电学和磁学性质研究
直接费用：160.00万元
项目起止年月：2019年01月至2021年12月
同时，国际合作者：莫斯科大学物理系Alexander Pyatakov教授、尼赫鲁高等科学研究中心A. Sundaresan教授也分别获得俄罗斯、印度国家政府重点资助。

National Research Foundation
Department of Science & Technology
Ministry of Science & Technology
Government of India
science & technology
Department: Science and Technology
REPUBLIC OF SOUTH AFRICA
RUSSIAN FOUNDATION FOR BASIC RESEARCH
RFBR
中华人民共和国科学技术部
Ministry of Science and Technology of the People's Republic of China
CNPq
Conselho Nacional de Desenvolvimento Científico e Tecnológico
FASIE
NSFC





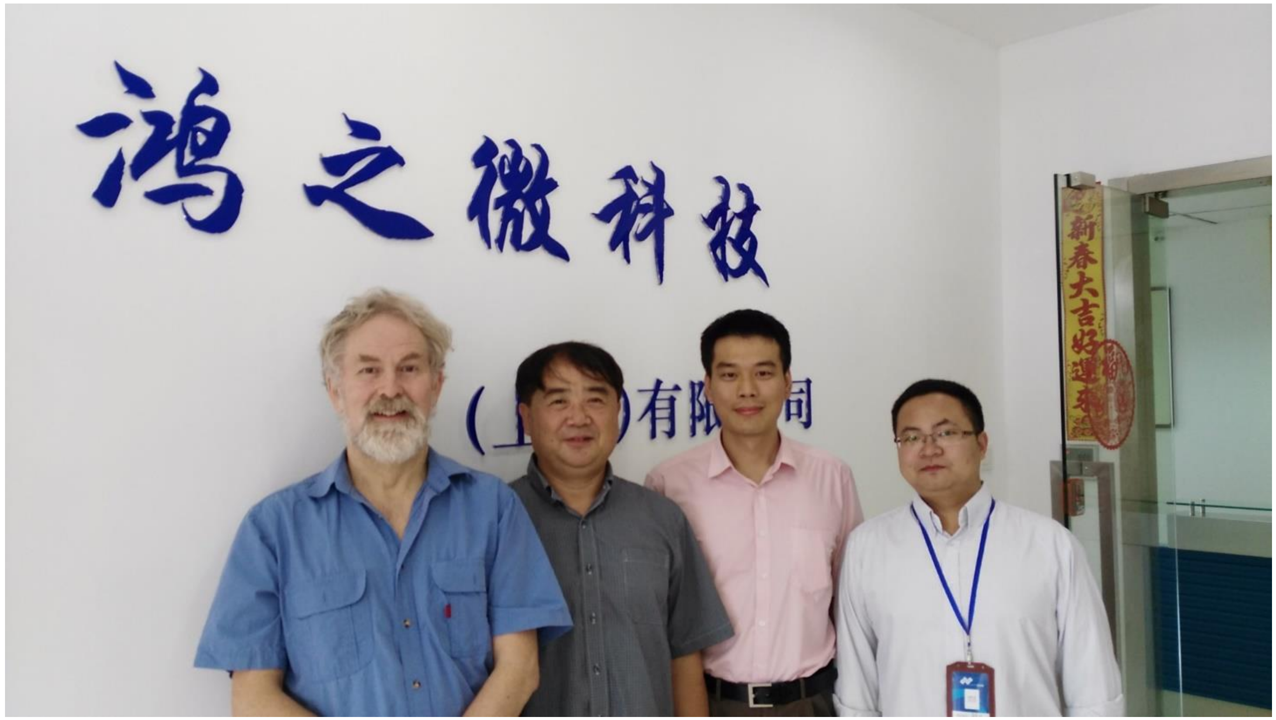
产学研结合

鸿之微科技（上海）股份有限公司

- 成立：2014年9月15日；注册资金：1187.5356万元；所在地：上海浦东；
- 核心业务：开发、推广材料设计、器件模拟计算软件及相关服务；
- 2016年完成股改，12月在上海股权托管交易中心科技创新板完成挂牌，公司治理完成规范化的飞跃。
- 2017年1月完成A轮千万级融资，投资方为新疆投资发展集团旗下基金。
- 2017年8月，与上海科技创业投资股份有限公司交换了投资意向协议，顺利展开了A+轮融资合作。

Industrial connections to HongZhiWei company

Yin Wang is General Manager



Jeffrey Reimers (杰夫)
上海大学全职教授
澳大利亚科学院士
鸿之微顾问科学家

Hong Guo (郭鸿)
上海大学自强教授
加拿大科学院士
鸿之微创始人

Wei Ren (任伟)
上海大学教授
东方学者跟踪
鸿之微高级科学家复旦大学博士

CEO Ronggen Cao
(曹荣根)
鸿之微董事长