Surface Bonding



样品	对称 COO/cm⁻¹	反对称 COO/cm ⁻¹	差值
100Ce	1440		
10Co	1440		
20Co	1440		









Co-K edge- XAFS



	shells	CN	R (Å)	$\sigma^2 (10^{-3} \text{ Å}^2)$
CeCo6	Со-О	6.3	2.03	6.7
	Co–Ce	1.9	3.31	14.5
CeCo14	Со-О	6.6	2.04	7.9
	Co–Ce	1.7	3.31	15.3



Ce L_3 XAFS

	shells	CN	R (Å)	$\sigma^2 (10^{-3} \text{ Å}^2)$
CeCo0	Ce–O1	6.3	2.33	6.7
	Ce–Ce	8.7	3.82	6.5
	Ce–O2	9.4	4.49	4.3
CeCo6	Ce–O1	5.9	2.32	7.2
	Ce–Ce	7.2	3.83	5.1
	(93.7%)			
	Се-Со	1.9	3.31	14.5
	(6.3%)			
	Ce–O2	5.9	4.46	6.8
CeCo14	Ce–O1	6.2	2.33	8.3
	Ce–Ce	7.4	3.83	5.3
	(85.7%)			
	Ce–Co	1.7	3.31	15.3
	(14.3%)			
	Ce–O2	5.4	4.46	7.0



Scheme of synthesis of monodisperse cobalt doped ceria

Nan Qiu, Jing Zhang, Takeshi Hashishin, Satoshi Ohara , Ziyu Wu RSC Advances RSC Adv.4,16033-16038

Surface and Interface Engineering in Nanocrystals For Enhanced Catalysis Properties



400 °C for 5 hours

Nano Lett. 2011, 11, 361-364

Before and After Calcined





	质量/ <i>mg</i>	面积	CO消耗量	${ m O}_2\mu mol/{ m g}$
			/mmol	
CuO	30.2	150990.8	0.3775	-
CeCo0	50.0	13682.43	0.0341	0.34
CeCo6	50.0	44656.22	0.1116	1.11
CeCo14	50.0	78755.21	0.1969	1.97



XRD

Co XAFS



Co的结构参数

	shells	CN	R (Å)	σ² (10 ⁻³ Ų)
Co ₃ O ₄	Co-O	6	1.89	-
	Co-Co1	6	2.86	-
	Co-Co2	6	3.35	-
CeCo6	Co-O	3.8	1.91	6.9
	Co-Co	0.4	2.82	2.0
	Co-Ce	1.1	3.75	6.8
CeCo14	Co-O	4.2	1.92	5.1
	Co-Co1	2.1	2.86	4.1
	Co-Co2	2.7	3.38	6.3

Ce XAFS



Ce的结构参数

	shells	CN	R (Å)	$\sigma^2 (10^{-3} \text{ Å}^2)$
CeO ₂	Ce–O	8*	2.34	1.9
CeCo0	Ce–O	7.1	2.34	3.7
CeCo6	Ce–O	5.2	2.33	2.9
CeCo14	Ce–O	4.9	2.33	2.9



Peculiar surface-interface properties of nanocrystalline ceria-cobalt oxides with enhanced oxygen storage capacity. Phys.Chem.Chem.Phys. Qiu N, Zhang J*, Wu ZY 2014, 16, 22659-22664

原位在线结构分析

纳米粒子的生长动力学过程







金属熔体中原子间距负膨胀现象

PNAS

Negative expansions of interatomic distances in metallic melts

Hongbo Lou^a, Xiaodong Wang^{a,1}, Qingping Cao^a, Dongxian Zhang^b, Jing Zhang^c, Tiandou Hu^c, Ho-kwang Mao^{a,d,e,1}, and Jian-Zhong Jiang^{a,f,1}

^aInternational Center for New-Structured Materials and Laboratory of New-Structured Materials, Department of Materials Science and Engineering, ^bState Key Laboratory of Modern Optical Instrumentation, and ^fState Key Laboratory of Silicon Materials, Zhejiang University, Hangzhou 310027, People's Republic of China; ^cBeijing Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, People's Republic of China; ^dCenter for High Pressure Science and Technology Advanced Research, Shanghai 201203, People's Republic of China; and ^eGeophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015







Synchrotron Radaition Instrument

Hongbo Lou et al., Negative expansions of interatomic distances in metallic melts, *PNAS* 2013, 110, 10068-10072.

高温超导体的同位素效应 <u>Scientific Reports</u> 和局域晶格动力学 Wangsheng Chu et al., Scientific Reports, 3, 1750, 2013.

Iron Isotope Effect and Local Lattice Dynamics in the (Ba, K)Fe₂As₂ Superconductor Studied by Temperature-Dependent EXAFS

Wangsheng Chu^{1,2}, Jie Cheng^{1,2}, Shengqi Chu², Tiandou Hu², Augusto Marcelli^{4,1}, Xianhui Chen³ & Ziyu Wu^{1,2}

¹National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, P.R. China, ²Beijing Synchrotron Radiation Facility, Institute of High EnergyPhysics, Chinese Academy of Sciences, Beijing 100049, P.R. China, ³Hefei National Laboratory for Physical Science at Microscale and Department of Physics, University of Science and Technology of China, Hefei 230026, China, ⁴Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, 00044 Frascati, Italy.



LowTemperature Cell

Table 1 | Values of local static distortions and Einstein temperatures associated to the As-Fe and Fe-Fe bonds in the 54 Fe- and 56 Fe-samples

bonds	Isotope	σ_0^2 (Å ²)	Т _Е (К)	α
As-Fe	⁵⁴ Fe ⁵⁶ Fe	$\begin{array}{c} 0.0025 \pm 0.0002 \\ 0.0024 \pm 0.0002 \end{array}$	331.5 ± 2.0 327.1 ± 2.0	0.37
Fe-Fe	⁵⁴ Fe ⁵⁶ Fe	$\begin{array}{c} 0.0056 \pm 0.0002 \\ 0.0053 \pm 0.0002 \end{array}$	169.0 ± 1.0 166.5 ± 1.0	0.41

Analysis Results

环境领域应用实例: 在鱼中汞的化学形态





Fig. 1. Comparison of the Hg L_{III} near-edge spectra of swordfish with selected solution spectra. The points show the spectrum of the fish; the solid lines show the spectra of aqueous solutions of standard species, as follows: (A) CH₃HgS(Cys), (B) CH₃HgCl, (C) Hg²⁺ (Hg(NO₃)₂ solution), and (D) Hg(SR)₂, (E) [Hg(SR)₄]²⁻.





从旗鱼的肌肉组织中检测到的汞

Hugh H. Harris,* Ingrid J. Pickering,† Graham N. George†‡ SCIENCE VOL 301 29 AUGUST 2003, 1203

植物修复技术

Implication of mercury speciation in thiosulfate-induced plants



中国科学院地球化学研究所冯新斌研究员与北京同步辐射XAFS课题组合作,通过研究植物体中化合物与汞结合的特点以及富集特征。发现利用硫代硫化物辅助植物修复可以有效提高植物修复效率,并显著降低汞污染土壤中氧化态汞和有机结合态汞的含量。而且土壤中的汞吸收到植物体后,主要是以一种类似黑色硫化汞的形态存在。

Wang J X et al Environ. Sci.Technol. 2012,46, 5361



中国土壤修复专家正在试验砷、铜、锌等重金属污染土壤的植物修复技术,通过在 矿区及其周边重金属污染土地种植超富集植物,吸收土壤中对人体有害的重金属物 质。(Huang Z C et al Environ. Sci.Technol. 2008,42(14) 5106)





临床实践证明全反式维甲酸 和三氧化二砷联合应用可以成功 地治疗全反式维甲酸耐药复发的 APL患者,APL成为第一种基本可 以被治愈的急性髓细胞性白血病。 但是三氧化二砷的直接分子靶点 和分子机理是什么一直是一个谜 团。

三氧化二砷(As₂O₃),俗称砒霜,剧毒,即 古代所指的"鹤顶红"。同时也是一种中药, 在中国古代医书中就有对As₂O₃治疗肿瘤等 一些疾病的记载。

经过20世纪后期的医学研究,发现了通过静脉注射 砒霜中提取出的三氧化二砷药剂成功治疗急性早幼 粒细胞性白血病(APL)的成功个案。

APL是一种特殊类型的急性髓细胞性白血病,具有特征性的PML-RAR癌蛋白,被认为是最为凶险的白血病之一。

上海交通大学医学院附属瑞金医院上海血液学研究所、医学基因组学国家重点实验室在三氧化二砷治疗急性早幼粒细胞性白血病(APL)分子机制的 研究中成功揭示: 癌蛋白PML-RAR是砷剂治疗APL的直接药物靶点。"全反式维甲酸+三氧化二砷"治疗白血病经典疗法,其针对同一癌蛋白上不同"特异 靶点"的"协同作战"机理得到了全面阐释。这一最新研究成果于2010年4月发表在国际权威杂志《科学(Science)》上。



这一研究成果不仅阐释了三氧化二砷治疗APL的药物分子靶点和分子机制,在医药学上将产生更加深远的意义。全反式维甲酸和砷剂分别靶相结合 到同一癌蛋白的不同区域而发挥协同作用,诱导白血病细胞分化凋亡,为肿瘤治疗的新策略提供了理论和实践依据。砷剂是一种具有2000多年历史记载 的古老中药,用现代科学手段揭示中药的分子作用机制,将促进中国科学家对祖国传统医学宝库进行深入探索和挖掘。

环境中的过渡金属氧化物 纳米粒子转化



Environmental Science & Technology

Jitao Lv et al., EST, 2012, 46(13):7215-7221.

Article pubs.acs.org/est

Dissolution and Microstructural Transformation of ZnO Nanoparticles under the Influence of Phosphate

3 Jitao Lv,[†] Shuzhen Zhang,*^{,†} Lei Luo,[†] Wei Han,[†] Jing Zhang,[‡] Ke Yang,[§] and Peter Christie^{||}

4 ⁺State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese

5 Academy of Sciences, Beijing 100085, China

⁶ [‡]State Key Laboratory of Synchrotron Radiation, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100039, 7 China

⁸ ⁸Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai, 201800, China

^{II}Agri-Environment Branch, Agri-Food and Biosciences Institute, Newforge Lane, Belfast BT9 5PX, United Kingdom



希土氧化物纳米粒子在植物体的转化 采用x-射线近边吸收光谱研究了纳米二氧化铈的生物转化,发现该纳米材料能够在黄瓜根 表面和细胞间隙形成磷酸铈纳米簇。为评价纳米二氧化铈的生态毒理和应用提供了重要 信息,拓展了x-射线吸收光谱学在纳米毒理学研究中的应用。该项研究成果发表在纳米科 学研究领域的权威杂志ACS Nano 2012,6(11),9943-9950



Ce L₃-edge XANES揭示纳米二氧化铈与黄瓜植株作用21天后,在根,茎,叶中 铈原子的化学形态

空间分辨技术研究金属元素在 植物体的分布和化学形态





Root anatomy



Leaf anatomy



Diagrams obtained from http://generalhorticultum.tamu.edu/actsup/anatomy/anatomy/timi

Anata - Ti Xylem average maps - LC-III (18%rxIIIe + 82% -Ti epidermis/cortex sp LC-in (13%nable + 87% Tiphicem spat 2 ------

Ti root maps (500ppm)

Maps acquired at 5.1Kev with a 200ms dwell time, a 5µm pixel and a 0.33x0.65µm beam size. White boxes are areas for XANES from root epidermis/contex (1) and philoem (2) acquired with a 50µm pinhole in unfocused mode.



range Intensity regions, the max for the red spots is ~8,000.



Ti in trichomes (500ppm)





t energy (eV)

Maps acquired at 5.1Kev with a 300ms dwell time, a 0.5µm pixel and a 0.33x0.65µm beam size. The circle represents the illuminated area for XANES acquisition in unfocused mode with a 50µm pinhole.

temperature map the scale is adjusted to 2.200 (raw intensity) in order to enhance the medium





Pt标准样品上任意样品区域内的吸收谱

采集不同能量下样品的投影数据,可以 获得任意像素点的微区吸收谱信息

共采集170个能量点图像,每个点曝光时间5ms,能 量扫描范围: 11.4Kev—11.8Kev,总用时2分钟

调制XAFS实验方法

Li₂MnO₃中Mn的k边近边调制谱与吸收谱对比

Nb标样调制谱与吸收谱R空间对比

✓调制吸收谱能突出常规测量中不明显的微结构,提高吸收谱测量的灵敏度。✓对高R部分即高配位层的微弱信号有放大作用,更利于对高配位层的研究。

推进XAFS实验方法和数据分析的规范和标准; 发展多种探测实验技术和样品环境平台; 应用多种同步辐射方法, 揭示多学科领域中的物质结构和性能的关联; 争取更为广泛的合作机会