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材料科学Materials Science

Stoichiometric reconstruction of the Al2O3(0001) surface

Al2O3（0001）表面的化学计量重构

▲ 作者：JOHANNA I. H ü TNER, ANDREA CONTI, DAVID KUGLER, FLORIAN MITTENDORFER, GEORG KRESSE, MICHAEL SCHMID, ET AL.

▲链接：

https://www.science.org/doi/10.1126/science.adq4744

▲摘要：

材料的宏观特性源于基本的原子尺度细节，但对于绝缘体来说，解析表面结构仍是一个挑战。

研究组使用具有原子定义尖端的非接触原子力显微镜对α-氧化铝（α-Al2O3）的（0001）基面进行了成像。表面形成了一个复杂的（√31 × √31）R±9°重构。单个氧和铝表面原子的横向位置直接源自实验；研究组通过计算模型确定了其与底层晶体块的连接方式。

在重构之前，表面Al原子呈不利的三重平面配位；重构实现了与亚表面O的再杂化，从而获得极大能量增益。重构表面仍保持Al2O3的化学计量比。

▲ Abstract：

Macroscopic properties of materials stem from fundamental atomic-scale details, yet for insulators, resolving surface structures remains a challenge. We imaged the basal (0001) plane of α – aluminum oxide (α-Al2O3) using noncontact atomic force microscopy with an atomically defined tip apex. The surface formed a complex (√31 × √31)R±9° reconstruction. The lateral positions of the individual oxygen and aluminum surface atoms come directly from experiment; we determined with computational modeling how these connect to the underlying crystal bulk. Before the restructuring, the surface Al atoms assume an unfavorable, threefold planar coordination; the reconstruction allows a rehybridization with subsurface O that leads to a substantial energy gain. The reconstructed surface remains stoichiometric, Al2O3.

能源科学Energy Science

Solvent-mediated oxide hydrogenation in layered cathodes

层状阴极中溶剂介导的氧化物氢化

▲ 作者：GANG WAN, TRAVIS P. POLLARD, LIN MA, MARSHALL A. SCHROEDER, CHIA-CHIN CHEN, ZIHUA ZHU, ET AL.

▲链接：

https://www.science.org/doi/10.1126/science.adg4687

▲摘要：

自放电和化学诱导的机械效应降低了嵌入式电致变色和电化学储能装置的日历寿命和循环寿命。在可充电锂离子电池中，阴极的自放电会随着时间的推移导致电压和容量损失。主流自放电模型聚焦于锂离子从电解液扩散至阴极的过程。

研究组展示了另一种途径，其中层状过渡金属氧化物阴极的氢化通过氢从碳酸盐溶剂转移到脱锂氧化物诱导自放电。在自放电阴极中，他们进一步观察到质子和锂离子浓度梯度负相关，这有助于脱锂阴极中化学和结构的异质性，从而加速降解。

在脱锂阴极中发生的氢化会影响层状阴极的化学-机械耦合以及锂离子电池的日历寿命。

▲ Abstract：

Self-discharge and chemically induced mechanical effects degrade calendar and cycle life in intercalation-based electrochromic and electrochemical energy storage devices. In rechargeable lithium-ion batteries, self-discharge in cathodes causes voltage and capacity loss over time. The prevailing self-discharge model centers on the diffusion of lithium ions from the electrolyte into the cathode. We demonstrate an alternative pathway, where hydrogenation of layered transition metal oxide cathodes induces self-discharge through hydrogen transfer from carbonate solvents to delithiated oxides. In self-discharged cathodes, we further observe opposing proton and lithium ion concentration gradients, which contribute to chemical and structural heterogeneities within delithiated cathodes, accelerating degradation. Hydrogenation occurring in delithiated cathodes may affect the chemo-mechanical coupling of layered cathodes as well as the calendar life of lithium-ion batteries.

人工智能Artificial Intelligence

Durably reducing conspiracy beliefs through dialogues with AI

通过与AI的对话持续减少阴谋论

▲ 作者：THOMAS H. COSTELLO, GORDON PENNYCOOK AND DAVID G. RAND

▲链接：

https://www.science.org/doi/10.1126/science.adq1814

▲摘要：

阴谋论的信徒臭名昭著地顽固。有影响力的假设提出，阴谋论满足了重要的心理需求，从而抵制了反证。然而，先前在纠正阴谋论信念方面的失败可能是由于反证不够令人信服和具有针对性。

为了评估这种可能性，研究组利用生成式人工智能的发展，让2190名阴谋论者与GPT-4 Turbo进行了个性化的循证对话。干预减少了约20%的阴谋论信念。这种影响在2个月后仍然存在，并在广泛的阴谋论中得到推广，甚至在信仰根深蒂固的参与者中也存在。

尽管对话集中在单个阴谋上，但其削弱了对不相关阴谋的信念，并改变了与阴谋相关的行为意图。这些发现表明，如果有足够令人信服的证据，许多阴谋论信徒可以转变他们的观点。

▲ Abstract：

Conspiracy theory beliefs are notoriously persistent. Influential hypotheses propose that they fulfill important psychological needs, thus resisting counterevidence. Yet previous failures in correcting conspiracy beliefs may be due to counterevidence being insufficiently compelling and tailored. To evaluate this possibility, we leveraged developments in generative artificial intelligence and engaged 2190 conspiracy believers in personalized evidence-based dialogues with GPT-4 Turbo. The intervention reduced conspiracy belief by ~20%. The effect remained 2 months later, generalized across a wide range of conspiracy theories, and occurred even among participants with deeply entrenched beliefs. Although the dialogues focused on a single conspiracy, they nonetheless diminished belief in unrelated conspiracies and shifted conspiracy-related behavioral intentions. These findings suggest that many conspiracy theory believers can revise their views if presented with sufficiently compelling evidence.

化学Chemistry

Characterization of a Lewis adduct in its inner and outer forms

路易斯加合物内外层形态的表征

▲ 作者：WEI-CHUN LIU AND FRAN Ç OIS P. GABBA Ï

▲链接：

https://www.science.org/doi/10.1126/science.adp7465

▲摘要：

双分子反应的入口通道有时涉及形成作为弱结合、短暂中间体的外层配合物。

研究组在一个系统中描述了这种外层配合物，该系统模拟了氧化膦路易斯碱与正碳离子路易斯酸的双分子C-O成键反应。晶体学研究表明，外层形态的C-O距离比最终形态或内层形态的C-O距离高出1.1埃。

当系统对两种形式的配合物（对应于相应势能面上的最小值）进行采样时，C-O键从外层配合物的次级相互作用转换到内层配合物的配位键。这种现象被用作稳定占吨翁基光氧化还原催化剂的功能特征。

▲ Abstract：

The entrance channel of bimolecular reactions sometimes involves the formation of outer complexes as weakly bound, fleeting intermediates. Here, we characterize such an outer complex in a system that models the bimolecular, C-O bond – forming reaction of a phosphine oxide Lewis base with a carbenium Lewis acid. Crystallographic studies show that the C-O distance in the outer form exceeds that of the final or inner adduct by 1.1 angstroms. As the system samples the two forms of the complex, which correspond to minima on the corresponding potential energy surface, the C-O linkage switches from a secondary interaction in the outer complex to a dative bond in the inner complex. This phenomenon is harnessed as a functional feature to stabilize xanthylium-based photoredox catalysts.

地球科学Earth Science

Mega El Ni ñ oinstigated the end-Permian mass extinction

超级厄尔尼诺引发了二叠纪末期大灭绝

▲ 作者：YADONG SUN, ALEXANDER FARNSWORTH, MICHAEL M. JOACHIMSKI, PAUL B. WIGNALL, LEOPOLD KRYSTYN, DAVID P. G. BOND, ET AL.

▲链接：

https://www.science.org/doi/10.1126/science.ado2030

▲摘要：

二叠纪末期物种大灭绝的最终原因是一个备受争议的话题。

研究组使用多代理和古气候建模方法来建立一个统一的理论，阐明了盘古大陆对导致灭绝状态的长期和加剧的厄尔尼诺事件的高度敏感性。在二叠纪晚期，随着二氧化碳的大气分压从约410 ppm增加到860
ppm（百万分之一），经向翻转环流崩溃，哈德利环流收缩，厄尔尼诺现象增强。

随之而来的毁林、珊瑚礁消亡和浮游生物危机标志着一场连锁环境灾难的开始。碳固存的减少引发了正反馈，产生了一个更温暖的温室，从而增强了厄尔尼诺现象。气候变化加剧和平均状态变暖的复合效应导致了灾难性但跨时性的陆地和海洋损失。

▲ Abstract：

The ultimate driver of the end-Permian mass extinction is a topic of much debate. Here, we used a multiproxy and paleoclimate modeling approach to establish a unifying theory elucidating the heightened susceptibility of the Pangean world to the prolonged and intensified El Ni ñ oevents leading to an extinction state. As atmospheric partial pressure of carbon dioxide doubled from about 410 to about 860 ppm (parts per million) in the latest Permian, the meridional overturning circulation collapsed, the Hadley cell contracted,

and El Ni ñ os intensified. The resultant deforestation, reef demise, and plankton crisis marked the start of a cascading environmental disaster. Reduced carbon sequestration initiated positive feedback, producing a warmer hothouse and, consequently, stronger El Ni ñ os. The compounding effects of elevated climate variability and mean state warming led to catastrophic but diachronous terrestrial and marine losses.

A rockslide-generated tsunami in a Greenland fjord rang Earth for 9 days

格陵兰峡湾山体滑坡引发的海啸使地球连震九天

▲ 作者：KRISTIAN SVENNEVIG, STEPHEN P. HICKS, THOMAS FORBRIGER, THOMAS LECOCQ, RUDOLF WIDMER-SCHNIDRIG, ANNE MANGENEY, ET AL.

▲链接：

https://www.science.org/doi/10.1126/science.adm9247

▲摘要：

气候变化使极地地区越来越容易发生大型山体滑坡。格陵兰岛（Kalaallit Nunaat）最近发生了海啸山体滑坡，但峡湾东部未报道发生。

2023年9月，研究组探测到一个源自东格陵兰岛、为期9天、全球10.88毫赫（92秒）单色超长周期（VLP）地震信号的出现。在该研究中，他们揭示了这一事件是如何开始的，冰川变薄引发25×106立方米的岩冰雪崩坠入迪克森峡湾，导致了200米高的海啸。

模拟表明，海啸稳定成一个7米高的长时间湖震，其频率（11.45毫赫）和缓慢的振幅衰减与地震信号几乎相同。一个最大振幅为5×1011牛顿的振荡峡湾横向单力再现了地震振幅及其相对于峡湾的辐射模式，证明了湖震如何直接引起长达9天的地震信号。该研究结果强调了气候变化如何在冰冻圈、水圈和岩石圈之间引发级联危险反馈。

▲ Abstract：

Climate change is increasingly predisposing polar regions to large landslides. Tsunamigenic landslides have occurred recently in Greenland (Kalaallit Nunaat), but none have been reported from the eastern fjords. In September 2023, we detected the start of a 9-day-long, global 10.88-millihertz (92-second) monochromatic very-long-period (VLP) seismic signal, originating from East Greenland. In this study, we demonstrate how this event started with a glacial thinning – induced rock-ice avalanche of 25 × 106 cubic meters plunging into Dickson Fjord, triggering a 200-meter-high tsunami. Simulations show that the tsunami stabilized into a 7-meter-high long-duration seiche with a frequency (11.45 millihertz) and slow amplitude decay that were nearly identical to the seismic signal. An oscillating, fjord-transverse single force with a maximum amplitude of 5 × 1011 newtons reproduced the seismic amplitudes and their radiation pattern relative to the fjord, demonstrating how a seiche directly caused the 9-day-long seismic signal. Our findings highlight how climate change is causing cascading, hazardous feedbacks between the cryosphere, hydrosphere, and lithosphere.

作者：未玖 来源：科学网微信公众号