

Quantification of topological spin chiral textures

Scientific Achievement

We conducted a quantitative measurement of chiral spin structure of domain-walls by developing a Lorentz electron microscopy method via Fresnel propagator that allows us to image weak contrast of three-dimensional spin arrangement.

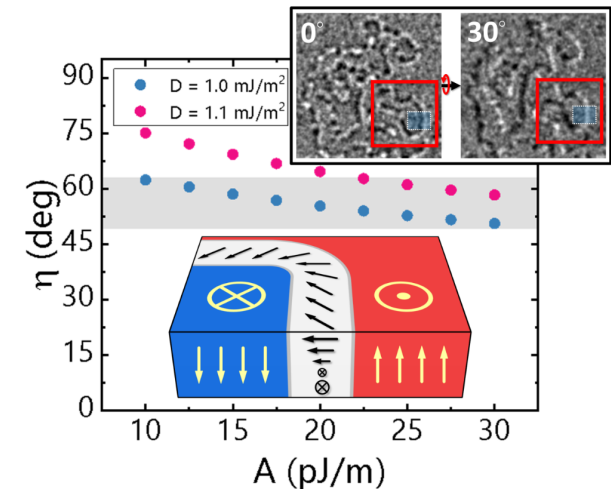
Significance and Impact

The approach can be used to measure traditionally invisible spin contrast and topological magnetic chiral textures in complex multilayer systems driven by Dzyaloshinskii-Moriya interactions (DMI).

Research Details

- We developed formulism of electron wave propagation to quantify for the first time the Bloch/Néel mixed character and the domain wall width in topological Pd/Co multilayer system.
- Correlating micromagnetic simulations we derived the crucial material parameters, including the strength of the DMI and magnetic exchange stiffness, for spintronic device applications.

Garlow, JA., Pollard, SD., Beleggia, M., Dutta, T., Yang, H., Zhu, Y., “Quantification of mixed Bloch/Néel topological spin textures stabilized by the Dzyaloshinskii–Moriya interaction in Co/Pd multilayers”, *Phys. Rev. Lett.*, 122, 237201 (2019).



Characteristic Bloch/Neel angle η as a function of exchange stiffness A for two values of Dzyaloshinskii-Moriya interaction D . The shaded region marks the experimentally measurement. Top-right panels show chiral domain wall contrast at zero and 30 degree sample tilt from a multilayer stack of MgO(2 nm)/Pt(4 nm)/Co(0.7 nm)/[Pd(0.5 nm)/Co(0.7 nm)]₁₀/Pt(4 nm). The schematic depicts the spin arrangement of the topological chiral domain wall.



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Nematic order and lattice dynamics in FeSe superconductor

Scientific Achievement

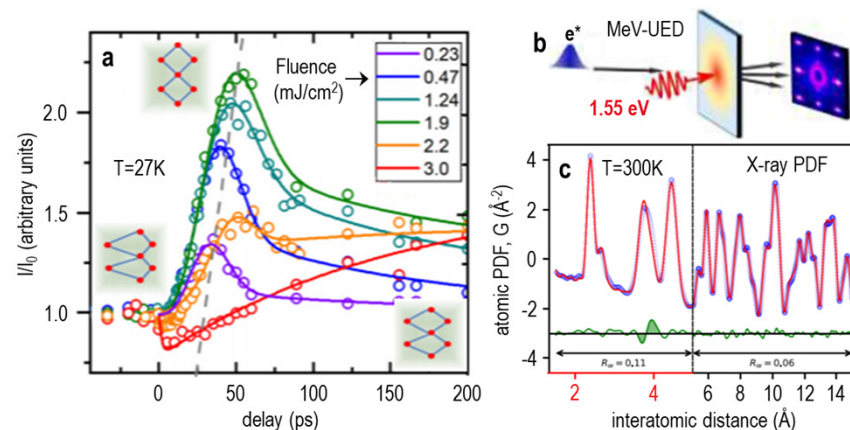
We probe nonequilibrium lattice interactions with electronic degrees of freedom in superconductor and reveal surprising atomic distortion as a response to local nematicity.

Significance and Impact

The observed structural response sheds light on the formation of the nematic phase due to the imperfect ordering of orbital-degeneracy-lifted precursor nematic fluctuations, significantly advancing our understanding of nematicity and superconductivity.

Research Details

- Ultrafast electron diffraction (UED) was used to investigate lattice response to local nematicity and x-ray pair distribution function was used to quantify atomic distortions.
- The distortions are present at temperatures both below and above the nematic phase transition and photoexcitation suppresses the electronic fluctuations induced local lattice distortions.



(a) Dynamics of (080) Bragg peaks as a function of time delay at different excitation fluences (indicated in the legend). Open circles are the experimental data and solid lines are the fits. Insets show schematics of unequal atomic bonds at the corresponding time intervals [1]. (b) Sketch of the UED setup used. (c) Experimental X-ray PDF signature of local nematic fluctuations at 300 K temperature, well above the low temperature ordered nematic state in tetragonal FeSe (nematic transition is at $T_S=90$ K). This precursor state is evidenced in the structure through a failure of the tetragonal model (red line) to explain 300K data (blue circles) on a short length scale, as revealed by the difference curve (green line)[2].

[1] T. Konstantinova, L. Wu, M. Abeykoon, R. J. Koch, A. F. Wang, R. K. Li, X. Shen, J. Li, J. Tao, I. A. Zaliznyak, C. Petrovic, S. J. L. Billinge, X. J. Wang, E. S. Bozin, and Y. Zhu, Photoinduced dynamics of nematic order parameter in FeSe, *Physical Review B, Rapid comm. Editors' suggestion*, **99**, 180102(R) (2019).

[2] R. J. Koch, T. Konstantinova, M. Abeykoon, A. Wang, C. Petrovic, Y. Zhu, E. S. Bozin, and S. J. L. Billinge, Room temperature local nematicity in FeSe superconductor, *Phys. Rev. B, Rapid comm. Editors' suggestion*, **100**, 020501(R) (2019).

The origin of second order modulation in charge-lattice coupled oxides

Scientific Achievement

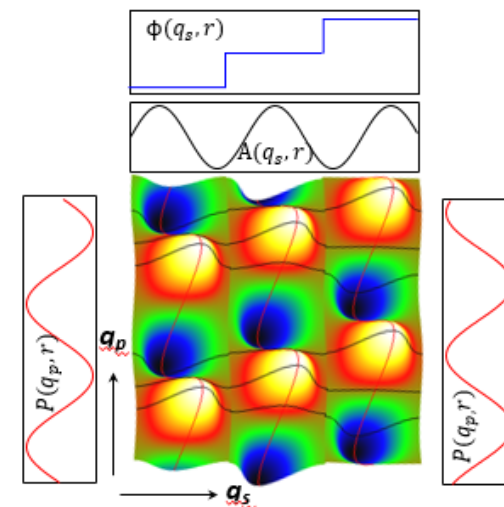
Atomic scale characterization revealed a new type of structural modulation originated from the periodic discontinuity of lattice displacement induced by valence change of the interstitial oxygen atoms in a hole-doped multiferroic $\text{LuFe}_2\text{O}_{4+\delta}$.

Significance and Impact

Entanglement between electron degree of freedom and lattice singularity yields an intertwined phase and amplitude variation in a modulation wave. The ability to analyze such a wave advances our understanding of the nature of singularity and modulation in condensed matter.

Research Details

- Atomically resolved imaging and electron energy-loss spectroscopy as well as diffraction analysis in 5-dimension enable us to identify the origin of the lattice singularity and entangled charge and lattice orders.
- Density function theory verifies the doped oxygen interstitials causes the intertwined modulation in the system.



Unlike traditional structure modulation where amplitude and phase of the wave modulation function is constant, a new type of modulation due to the charge and lattice singularity was observed and analyzed in hole doping $\text{LuFe}_2\text{O}_{4+\delta}$. The phase and amplitude of the primary wave $P(q_p, r)$ (red sine wave) are modulated by a phase function (blue step function) and an amplitude function (black sine wave), forming a new secondary modulation: $M(q_p, q_s, r) = A(q_s, r) \sin[2\pi q_p \cdot r + \Phi(q_s, r)]$. Color represents the amplitude of the wave function. q is the wave vector and r the atom position.

Deng, S.; Wu, L.; Cheng, H.; Zheng, J-C.; Cheng, S.; Li, J.; Wang, W.; Shen, J.; Tao, J.; Zhu, J.; Zhu, Y., "Charge-Lattice Coupling in Hole-Doped $\text{LuFe}_2\text{O}_{4+\delta}$: The Origin of Second-Order Modulation", Phys. Rev. Lett 122, 126401 (2019).

Spontaneous magnetic switching in a monolithic thin film

Scientific Achievement

Ability to image and understand unique macroscopic magnetic properties of single layer (monolithic) thin films via a three team collaboration (LSU, BNL, & Vanderbilt University) funded by DoE.

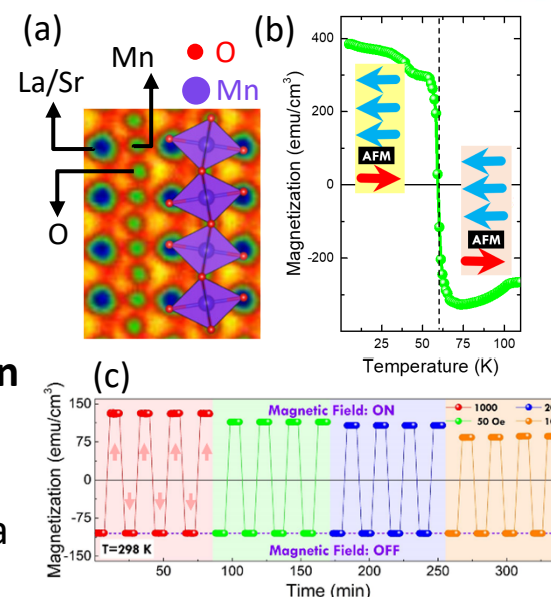
Significance and Impact

To achieve new functionalities, instead of multi-material heterostructuring, one can take advantage of substrate induced local structural modification to control physical properties of film that in addition to reducing the dimensionality, enhances functionality.

Research Details

- Monolithic thin films of $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ are epitaxially grown on a SrTiO_3 substrate (LSU) and studied using scanning transmission electron microscopy and spectroscopy (BNL).
- As shown by theory (Vanderbilt University) and experiment (LSU), the magnetic properties of the entire thin film are controlled by a single unit cell in proximity of the substrate.
- The interface driven modifications leads to magnetic reversal of entire thin film, that can be used as a magnetic switch (figure c).

M. Saghayezhian, Summayya Kouser, Zhen Wang, Hangwen Guo, Rongying Jin, Jiandi Zhang, Yimei Zhu, Sokrates T. Pantelides, and E. W. Plummer “Atomic-scale determination of spontaneous magnetic reversal in oxide heterostructures” *Proceedings of the National Academy of Sciences*, Accepted (2019).



(a) The Scanning electron microscope image of $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ revealing the octahedral structure. (b) The magnetization as a function of temperature (green curve) shows the total magnetization reversal due to antiferromagnetic coupling (AFM) at the interface. The two schematics show the magnetic moments orientation below (left) and above (right) reversal temperature (~ 65 K). (c) The AFM coupling creates magnetic switching functionality at room temperature, where the magnetic field aligns the moments and removing the field leads to spontaneous magnetic reversal. This behavior is shown for fields of different magnitudes.

Revealing “hidden” spin states by femtosecond optical manipulation

Scientific Achievement

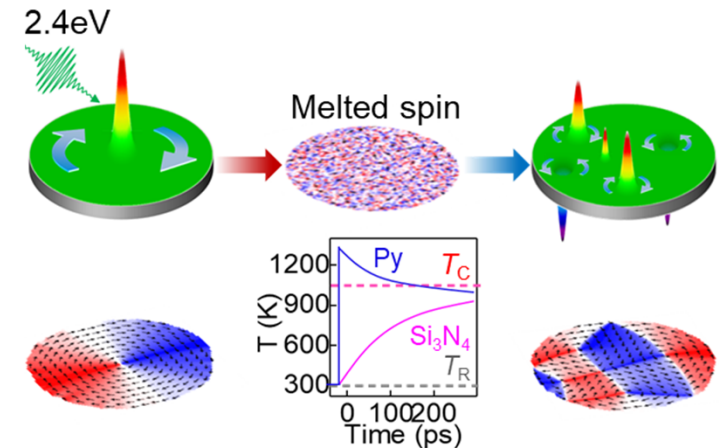
First in situ investigation with combined Lorentz phase electron microscopy and micromagnetic simulations reveal femtosecond-laser-pulse induced vortex switching behavior and “hidden” spin states confined in Permalloy disks.

Significance and Impact

The transient vortex behavior via optical quenching was never observed in traditional field and current induced vortex excitation, yielding a new paradigm of optical-assisted ultrafast spin-switching for vortex-based data recording.

Research Details

- Using ultrafast laser we melt and quench the spin states to generate new symmetric and unexpected “hidden” vortex states with different occurrence frequencies.
- The “hidden” states consist of new vortex-antivortex configurations that strictly conserve topological invariance.
- The geometry and edge shape of the disks strongly affect spin relaxation and its final states after the laser excitation.



Schematic of in situ study of transient spin phenomena in magnetic vortex systems under ultrafast fs-laser-pulse excitation and quenching. Top: a laser pulse transiently melts the spin configuration of the vortex system and then the melted spin system relaxes into various unexpected new spin states (hidden states) due to the extremely high quenching rate ($>10^{12}$ K/sec). Bottom: the corresponding in-plane spin configurations of the vortex where red and blue color represent the opposite spin direction. The middle panel shows the temperature evolution of the sample after a fs-laser-pulse excitation.

Fu, X., Pollard, S.D., Chen, B., Yoo, B.K., and Zhu, Y.,

“Optical Manipulation of Magnetic Vortex Visualized in situ by Lorentz Electron Microscopy”, *Sci. Adv.* **4**, aat3077 (2018)



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Direct imaging of interfacial electron transfer and superconducting pairing

Scientific Achievement

Cryo-interfacial characterization combined with electrical transport measurement of FeSe films on SrTiO_3 , via varying FeSe thickness, backgating and annealing, reveal the origin of the increase in superconducting transition temperature T_c .

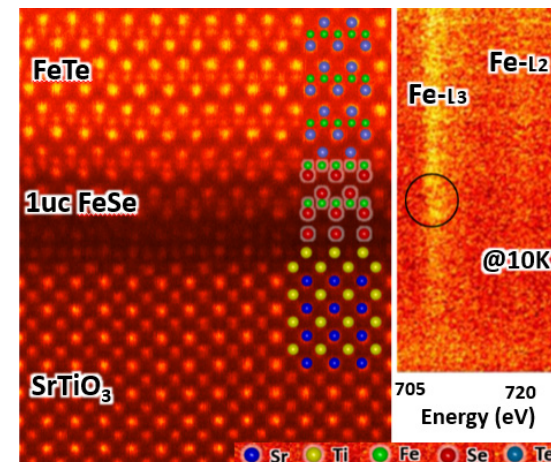
Significance and Impact

The T_c in 1uc FeSe on SrTiO_3 can be 10 times higher than its bulk counterpart. Understanding the origin of this increase can help understand the pairing mechanism, design and search for new high- T_c superconductors.

Research Details

- low-temperature EELS shows a blue shift of Fe-L edge within the first two atomic layers of FeSe due to the interfacial electronic band bending.
- positive backgating pulls electrons in FeSe closer to the interface and thus enhances their coupling to interfacial phonons and electron-electron interaction, yielding higher T_c .

Zhao, W., Li, M., Chang, C-Z., Jiang, J., Wu, L., Liu, C., Moodera, J.S., Zhu, Y.,* Chan, M.H.W., "Direct imaging of electron transfer and its influence on superconducting pairing at FeSe/ SrTiO_3 interface", *Sci. Adv.* **4**, eaao2682 (2018).



Left: atomic image of the 1 unit-cell (uc) superconducting FeSe on the SrTiO_3 substrate with 10uc FeTe as a capping layer. Unexpected interfacial atomic arrangement has been identified. Right: electron energy-loss spectroscopy mapping of the same area, showing the energy shift of the Fe-L₃ edge (marked by the circle) at the FeSe/ SrTiO_3 interface due to the electron transfer from SrTiO_3 to FeSe below the superconducting transition temperature.



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From hot electrons to acoustic phonons: direct observation of nonequilibrium energy flow in superconductor

Scientific Achievement

First observation with combined ultrafast electron diffraction (UED) and time-and angle-resolved photoelectron spectroscopy (tr-ARPES) revealed the path of nonequilibrium energy flow in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8\delta}$, a high- T_c cuprate superconductor

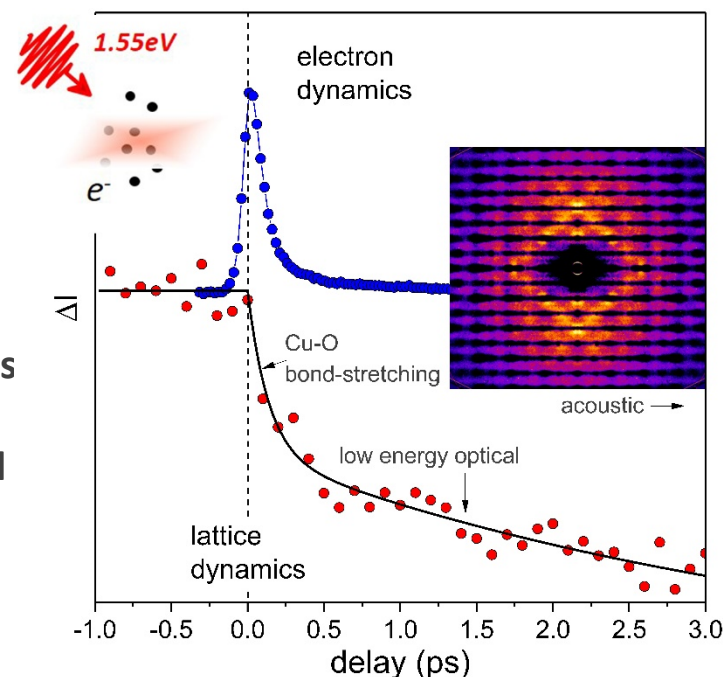
Significance and Impact

The role of the lattice in the electron relaxation in the cuprates is unequivocally identified. Nonthermal phonon distribution challenges the validity of temperature model commonly applied for similar strongly correlated systems.

Research Details

- tr-ARPES measurements of the electron dynamics at different parts of the Brillouin zone
- UED measurements of phonon dynamics with momentum-resolved information.
- separation of atomic motions, optical and acoustic phonons, based on electron diffuse scattering and Bloch-Wave calculations

T. Konstantinova, J.D. Rameau, A.H. Reid, O. Abdurazakov, L. Wu, R.K. Li, X. Shen, G. Gu, Y. Huang, L. Rettig, I. Avigo, M. Ligges, J. K. Freericks, A. H. F. Kemper, A. Dürr, U. Bovensiepen, P.D. Johnson, X. Wang, Y. Zhu, *Nonequilibrium electron and lattice dynamics of strongly correlated $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8\delta}$ single crystals*, **Science Advances** 2018; 4: eaap7427



Top: Dynamics of electrons above the Fermi level. Zero time corresponds to the arrival of the laser pulse (upper inset).

Bottom: Intensity of Bragg peaks. Phonons, responsible for the peak decay are marked at the corresponding characteristic time. The lower inset is the diffuse background formed by acoustic phonons at +180ps delay

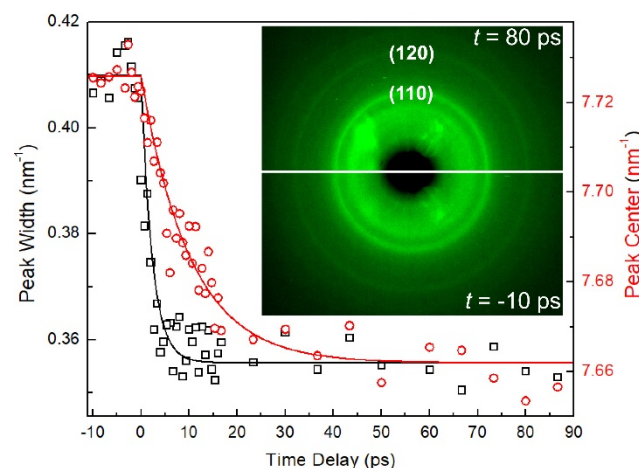
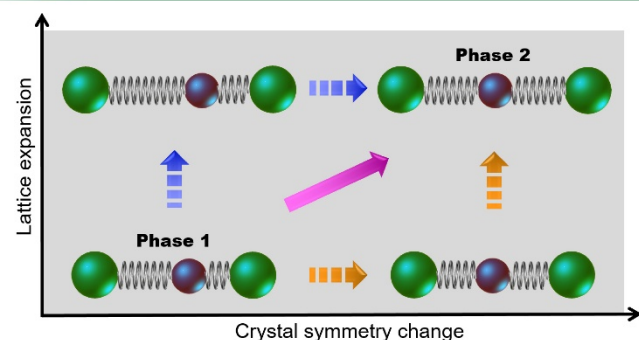


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Probing the pathway of structural phase transition



Upper: Schematic of the possible pathways of a structural transition involving symmetry breaking and lattice expansion in a 1D assembly of atoms.

Lower: The change of peak width and center for the (110) peak in the ultrafast-time domain measured from UED patterns shown in the inset.

Scientific Achievement

An experimental disentanglement of crystal symmetry breaking and volume change in the ultrafast-time domain, two order parameters that have long been considered to be “simultaneous”, during the phase transition in Cu₂S.

Significance and Impact

The work demonstrates a novel approach to separate the primary order parameter from secondary order parameters, which is essential to pin down the phase transition mechanisms.

Research Details

- Identified the transition pathway in Cu₂S that crystal symmetry changes first, followed by lattice expansion.
- Found the temporal characteristic of crystal symmetry change the same as in electronic structures.
- Revealed the transition mechanism in Cu₂S to be electron-phonon coupling.

Junjie Li, ... Jing Tao, Applied Physics Letters 113, 079902 (2018)

Work was performed at Brookhaven National Laboratory.

Lithium ionic diffusion in nanorods assisted by defects

Scientific Achievement

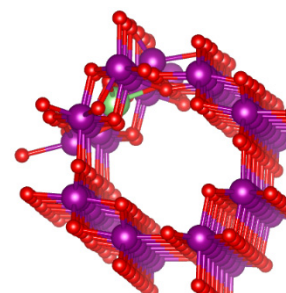
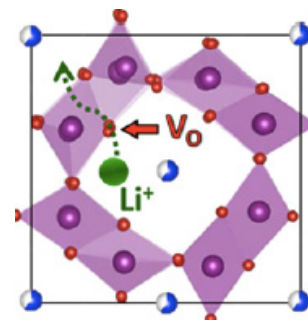
A collaboration among researchers from the m2M EFRC, the CMPMSD department at Brookhaven and the CFN used atomically resolved structural characterization and density functional theory calculations to establish the presence of a significant amount of oxygen vacancies near the surface of silver hollandite nanorod electrodes and to show that despite inherently one-dimensional tunnels internally, near surface oxygen defects can mediate three-dimensional ionic diffusion.

Significance & Impact

This new atomic-scale insight explains unexpected diffusion characteristics with potential for improving charge and discharge characteristics in nanostructured electrodes.

Research Details

CFN led theory and computation mapped out the pathways for lithium diffusion, demonstrating the role of oxygen vacancies to enable ionic transport through manganese oxide tunnel walls.



Top: Illustration of the 1D tunnel in silver hollandite and a schematic for lithium to diffuse through a tunnel wall. Bottom: Atomic scale model based on calculations for the transition state in which the lithium ion (green) occupies the space in the wall created by an oxygen divacancy.

"Revealing effect of oxygen vacancy & surface disorder on ionic transport in 1-dimensional tunneled structure"

Hu, X., Huang, J., Wu, L., Kaltak, M., Fernandez-Serra, M., Meng, Q., ..., Hybertsen, M.S., and Zhu, Y., Chemistry of Materials 30, 6124 (2018)

Imaging ordered defects by design

The Science

Defects exist in every material we live with and they can be as small as an atom. At microscopic level, the appearance of defects tends to be disordered, i.e., their positions are random and hard to predict. We discovered a method to synthesis materials in which the 2 dimensional defects (known as antiphase boundary) have well-defined positions and origin. The power of atomic-resolved electron microscopy allows us to directly visualize their atomic arrangements and unique properties and theory predicts how they interact with each other.

The Impact

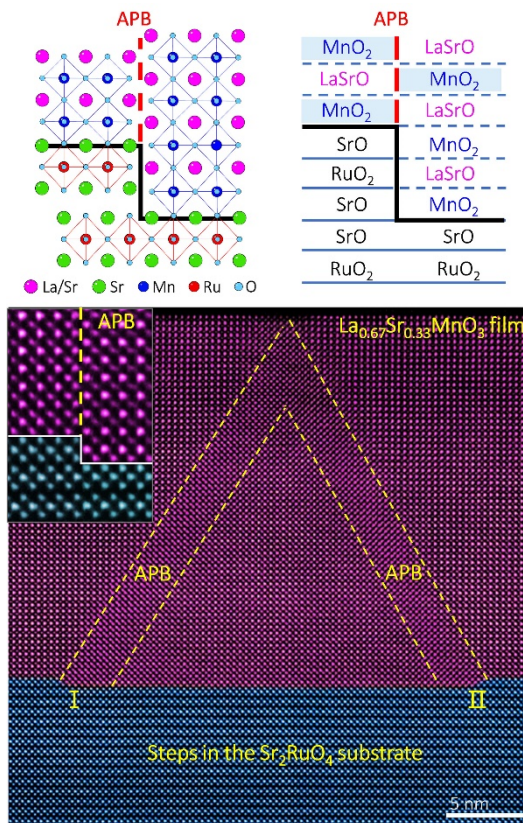
Our findings reveal a novel way to design ordered defects with known locations inside a crystal. Combined with atomic-resolved electron microscopy, our results offer the first glimpse of how to design defects to tailor the material's physical and mechanical performances.

Publication

Z. Wang et al. "Designing antiphase boundaries by atomic control of heterointerfaces", *Proceedings of National Academy of Science, U.S.A.* 115, 9485 (2018). [DOI: 10.1073/pnas.1808812115].

Related Links

PNAS commentary on the research: <http://www.pnas.org/content/115/38/9344>



Top is schematic image of the APB between the Sr_2RuO_4 substrate with a single step and the $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ film. The inset at bottom shows STEM image of a signal AFB, with a STEM image of two merged APBs.



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This work was primarily supported by the US Department of Energy (DOE) under Grant No. DOE DE-SC0002136.

LSU

Manipulation and symmetry breaking of topological defects

Scientific Achievement

First observations of topological defects with crystallographically forbidden but topologically allowed symmetries and their transformations.

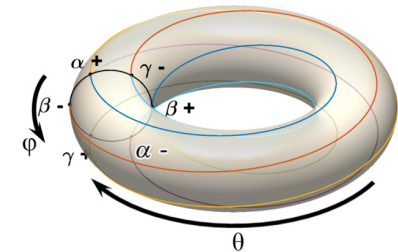
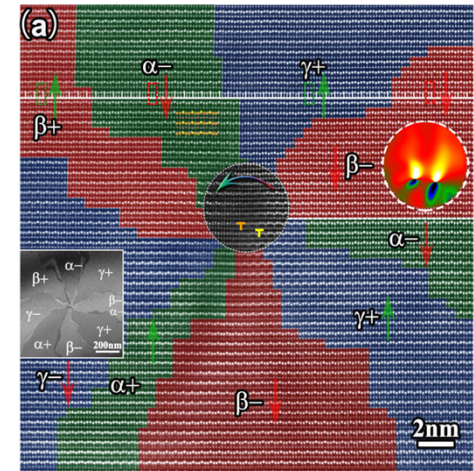
Significance and Impact

New route to unlock topological protection in technologically important multiferroics may provide new insights into topological defects.

Research Details

- Atomic resolution dipole mapping to reveal the origin of the transformations of 6-fold vortices into 2-, 4-, and 8-fold ones in the hexagonal manganite.
- Topological classification by Landau-based numerical simulation and homotopy group theory.

Cheng, Li, Han, Deng, Tan, Zhang, Zhu, and Zhu, “Topologically allowed nonsixfold vortices in a sixfold multiferroic material: observation and classification”, Phys. Rev. Lett. 118, 145501 (2017), highlighted on the journal cover.



Top: An 8-fold vortex core (circled region in the center) in hexagonal YMnO₃ observed by atomic resolution dipole mapping. Color corresponds to different vortex domains. The inset on the left and right shows the low-mag image and strain map of the core, respectively. Bottom: torus-like order-parameter space of the vortex revealed by Landau-based numerical calculations.



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NEWS RELEASE: Measuring the Charge of Electrons in a High-Temp Superconductor



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The following news release is being issued today by the U.S. Department of Energy's Brookhaven National Laboratory.

* * *

Measuring the Charge of Electrons in a High-Temp Superconductor

Scientists found a large concentration of electron pairs outside key temperature and energy ranges; this finding could inform the search for new materials that conduct electricity without resistance at unusually high temperatures

August 21, 2019

UPTON, NY—A team of scientists has collected experimental evidence indicating that a large concentration of electron pairs forms in a copper-oxide (cuprate) material at a much higher temperature than the "critical" one (T_c) at which it becomes superconducting, or able to conduct electricity without energy loss. They also detected these pairs way above the superconducting energy gap, or a range of energies that electrons cannot possess.

Their results, published today in the journal *Nature*, may point at a way to boost the superconducting properties of cuprates and to find new—and perhaps better—high-temperature superconductors (HTS). While cuprates and other HTS become superconducting at unusually high temperatures compared to conventional superconductors, they still require expensive cooling with liquid nitrogen to operate. Research aimed at understanding the mechanism behind high-temperature superconductivity could help scientists further raise T_c to an economically practical level at which large-scale applications, such as lossless power lines across the electric grid, could be enabled.

"If you don't know where to look, the phase space is infinite," said co-corresponding author Ivan Bozovic, group leader of the Oxide Molecular Beam Epitaxy Group [<https://www.bnl.gov/cmpmsd/mbe/>] in the Condensed Matter Physics and Materials Science (CMPMS) Division [<https://www.bnl.gov/cmpmsd/>] at the U.S. Department of Energy's (DOE) Brookhaven National Laboratory and professor of applied physics at Yale University. "Our measurement spectra directly revealed a high percentage of electron pairs well above the expected temperature and energy ranges. The exciting prospect now is to leverage this knowledge to enhance superconductivity in cuprates by chemically or physically tweaking some parameters, or to search for other strange metals in which such pairs could exist."

A mysterious electronic state

NEWS RELEASE: New Core-Shell Catalyst for Ethanol Fuel Cells



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Fri 2019-06-07 11:3

The following news release is being issued today by the U.S. Department of Energy's Brookhaven National Laboratory.

* * *

New Core-Shell Catalyst for Ethanol Fuel Cells

Greatly boosts efficiency of ethanol electro-oxidation, offering promise for liquid-fuel-cell-powered drones

June 7, 2019

UPTON, NY—Scientists at the U.S. Department of Energy's (DOE) Brookhaven National Laboratory and the University of Arkansas have developed a highly efficient catalyst for extracting electrical energy from ethanol, an easy-to-store liquid fuel that can be generated from renewable resources. The catalyst, described in the *Journal of the American Chemical Society*, steers the electro-oxidation of ethanol down an ideal chemical pathway that releases the liquid fuel's full potential of stored energy.

"This catalyst is a game changer that will enable the use of ethanol fuel cells as a promising high-energy-density source of 'off-the-grid' electrical power," said Jia Wang, the Brookhaven Lab chemist who led the work. One particularly promising application: liquid fuel-cell-powered drones.

"Ethanol fuel cells are lightweight compared to batteries. They would provide sufficient power for operating drones using a liquid fuel that's easy to refill between flights—even in remote locations," Wang noted.

Much of ethanol's potential power is locked up in the carbon-carbon bonds that form the backbone of the molecule. The catalyst developed by Wang's group reveals that breaking those bonds at the right time is the key to unlocking that stored energy.



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NEWS RELEASE: New Lens System for Brighter, Sharper Diffraction Images



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The following news release is being issued today by the U.S. Department of Energy's Brookhaven National Laboratory.

* * *

New Lens System for Brighter, Sharper Diffraction Images

Researchers from Brookhaven Lab designed, implemented, and applied a new and improved focusing system for electron diffraction measurements

April 25, 2019

UPTON, NY - To design and improve energy storage materials, smart devices, and many more technologies, researchers need to understand their hidden structure and chemistry. Advanced research techniques, such as ultra-fast electron diffraction imaging can reveal that information. Now, a group of researchers from the U.S. Department of Energy's (DOE) Brookhaven National Laboratory have developed a new and improved version of electron diffraction at Brookhaven's Accelerator Test Facility (ATF) [https://www.bnl.gov/atf/]—a DOE Office of Science User Facility that offers advanced and unique experimental instrumentation for studying particle acceleration to researchers from all around the world. The researchers published their findings [https://www.nature.com/articles/s41598-019-39208-z] in Scientific Reports, an open-access journal by Nature Research.

Advancing a research technique such as ultra-fast electron diffraction will help future generations of materials scientists to investigate materials and chemical reactions with new precision. Many interesting changes in materials happen extremely quickly and in small spaces, so improved research techniques are necessary to study them for future applications. This new and improved version of electron diffraction offers a stepping stone for improving various electron beam-related research techniques and existing instrumentation.

"We implemented our new focusing system for electron beams and demonstrated that we can improve the resolution significantly when compared to the conventional solenoid technique," said Xi Yang, author of the study and an accelerator physicist at the National Synchrotron Light Source II (NSLS-II), a DOE Office of Science User Facility at Brookhaven Lab. "The resolution mainly depends on the properties of light—or in our case—of the electron beam. This is universal for all imaging techniques, including light microscopy and x-ray imaging. However, it is much more challenging to focus the charged electrons to a near-parallel pencil-like beam at the sample than it would be with light, because electrons are negatively charged and therefore repulse one another. This is called the space charge effect. By using our new setup, we were able to overcome the space charge effect and obtain diffraction data that is three times brighter and two times sharper; it's a major leap in resolution."

NEWS RELEASE: Scientists Pinpoint Energy Flowing Through Vibrations in Superconducting Crystals



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Thu 2018-05-03 10:34

The following news release is being issued today by the U.S. Department of Energy's Brookhaven National Laboratory.

* * *

Scientists Pinpoint Energy Flowing Through Vibrations in Superconducting Crystals

Interactions between electrons and the atomic structure of high-temperature superconductors impacted by elusive and powerful vibrations

May 3, 2018

Manipulating the flow of energy through superconductors could radically transform technology, perhaps leading to applications such as ultra-fast, highly efficient quantum computers. But these subtle dynamics—including heat dispersion—play out with absurd speed across dizzying subatomic structures.

Now, scientists have tracked never-before-seen interactions between electrons and the crystal lattice structure of copper-oxide superconductors. The collaboration, led by scientists at the U.S. Department of Energy's (DOE) Brookhaven National Laboratory, achieved measurement precision faster than one trillionth of one second through a groundbreaking combination of experimental techniques.



"This breakthrough offers direct, fundamental insight into the puzzling characteristics of these remarkable materials," said Brookhaven Lab scientist Yimei Zhu, who led the research. "We already had evidence of how lattice vibrations impact electron activity and disperse heat, but it was all through deduction. Now, finally, we can see it directly."

The results, published April 27 in the journal Science Advances, could advance research into powerful, fleeting phenomena found in copper oxides—including high-temperature superconductivity—and help scientists engineer new, better-performing materials.

NEWS RELEASE: Surprising Discovery Could Lead to Better Batteries



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Fri 2018-01-12 14:18

The following news release is being issued today by the U.S. Department of Energy's Brookhaven National Laboratory.

* * *

Surprising Discovery Could Lead to Better Batteries

Scientists have observed how lithium moves inside individual nanoparticles that make up batteries. The finding could help companies develop batteries that charge faster and last longer.

January 12, 2018

UPTON, NY — A collaboration led by scientists at the U.S. Department of Energy's (DOE) Brookhaven National Laboratory has observed an unexpected phenomenon in lithium-ion batteries—the most common type of battery used to power cell phones and electric cars. As a model battery generated electric current, the scientists witnessed the concentration of lithium inside individual nanoparticles reverse at a certain point, instead of constantly increasing. This discovery, which was published on January 12 in the journal *Science Advances*, is a major step toward improving the battery life of consumer electronics.

"If you have a cell phone, you likely need to charge its battery every day, due to the limited capacity of the battery's electrodes," said Esther Takeuchi, a SUNY distinguished professor at Stony Brook University and a chief scientist in the Energy Sciences Directorate at Brookhaven Lab. "The findings in this study could help develop batteries that charge faster and last longer."

Visualizing batteries on the nanoscale

Inside every lithium-ion battery are particles whose atoms are arranged in a lattice—a periodic structure with gaps between the atoms. When a lithium-ion battery supplies electricity, lithium ions flow into empty sites in the atomic lattice.

"Previously, scientists assumed that the concentration of lithium would continuously increase in the lattice," said Wei Zhang, a scientist at Brookhaven's Sustainable Energy Technologies Department. "But now, we have seen that this may not be true when the battery's electrodes are made from nano-sized particles. We observed the lithium concentration within local regions of nanoparticles go up, and then down—it reversed."

NEWS RELEASE: Brookhaven Lab Materials Physicist Yimei Zhu Receives 2018 Distinguished Scientist Award from the Microscopy Society ...



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The following news release is being issued today by the U.S. Department of Energy's Brookhaven National Laboratory.

* * *

Brookhaven Lab Materials Physicist Yimei Zhu Receives 2018 Distinguished Scientist Award from the Microscopy Society of America Award recognizes his contributions to electron microscopy instrumentation and methods for understanding how complex atomic and electronic interactions impact the properties of materials

April 18, 2018

UPTON, NY—The Microscopy Society of America [<https://www.microscopy.org/>] (MSA) has selected Yimei Zhu—a senior physicist and leader of the Electron Microscopy and Nanostructure Group [<https://www.bnl.gov/cmpmsd/tem/>] in the Condensed Matter Physics and Materials Science Department at the U.S. Department of Energy's (DOE) Brookhaven National Laboratory—to receive the 2018 Distinguished Scientist Award for physical sciences. This award annually recognizes two senior scientists, one in the physical sciences and the other in biological sciences, for their long-standing record of achievement in the field of microscopy and microanalysis.

"I am extremely humbled by this recognition, the highest honor of the society, and to be selected among the most distinguished scientists in the field worldwide," said Zhu. "Four Nobel Laureates received the same award before winning the Nobel Prize: Ernst Ruska in 1985, Joachim Frank in 2003, Richard Henderson in 2005, and Jacques Dubochet in 2009. I strongly feel that my award is the result of not only my hard work, persistence, and curiosity about the inner world of matter but also my collaborations with colleagues and support from Brookhaven Lab and DOE over the past 30 years."

"Yimei Zhu has made significant contributions to advancing ultrafast electron diffraction instruments and developing fast direct-electron-detectors," said Molly McCartney, awards committee physical sciences co-chair. "Yimei's contributions to instrumentation and methods are extensive. His most highly recognized achievement is the successful imaging, at atomic resolution, of the atomic structure of bulk catalysts by detecting the secondary electron emission."



U.S. DEPARTMENT OF
ENERGY | Science

March 2017

Ultrafast Imaging Reveals the Electron's New Clothes

Scientists use high speed electrons to visualize “dress like” distortions in the atomic lattice

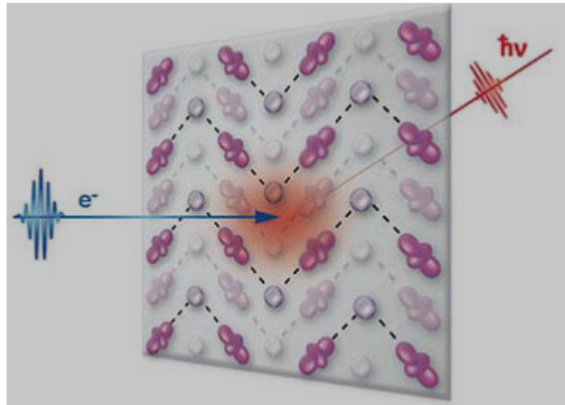


Image and caption courtesy of Brookhaven National Laboratory

Imaging atomic-scale electron-lattice interactions: A laser pulse (red beam coming from right) gives electrons in a manganese oxide a “kick” of energy while a high-energy electron beam (blue) probes the atomic structure. Circle- and rod-shaped blobs represent spherical and elongated electron clouds on the manganese atoms. The oxygen atoms (not shown) form regular and elongated octahedra around the manganese atoms. Varying the time delay between the pulse and the probe reveals-allows to directly measure time-resolved subtle shifts in atomic arrangements as the lattice responds to the kicked-up electrons. It reveals the motion of the electrons in the system being accompanied by the atomic lattice deformation it induces.

The Science

Knowing how electrons interact with the atomic lattice as they travel through a material is crucial for understanding properties such as electrical conductivity. Using ultrafast and ultrahigh-energy electron diffraction, scientists have demonstrated that the movement of electrons can drive deformations of their surrounding crystalline lattice, drastically altering the flow of electric current. This work provides strong evidence for the formation of polarons — a “quasiparticle” that arises from strong electron-lattice interactions.



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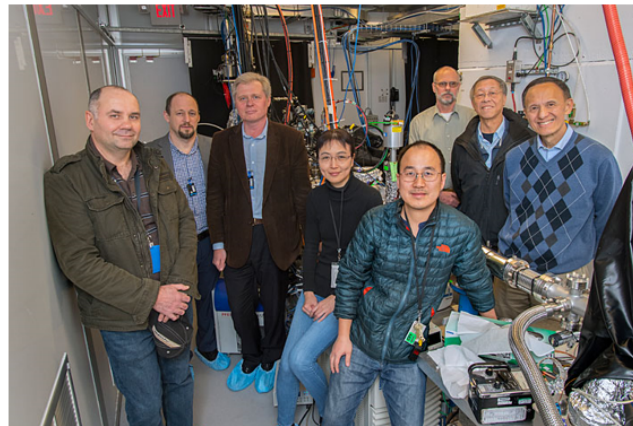
Contact: [Cara Laesch](#), (631) 344-8458, or [Peter Genzer](#), (631) 344-3174

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New Lens System for Brighter, Sharper Diffraction Images

Researchers from Brookhaven Lab designed, implemented, and applied a new and improved focusing system for electron diffraction measurements

April 25, 2019



Mikhail Fedurin, Timur Shaftan, Victor Smalyuk, Xi Yang, Junjie Li, Lewis Doom, Linhua Yu, and Yimei Zhu are the Brookhaven team of scientists that realized and demonstrated the new lens system for as ultra-fast electron diffraction imaging. [+ ENLARGE](#)

To design and improve energy storage materials, smart devices, and many more technologies, researchers need to understand their hidden structure and chemistry. Advanced research techniques, such as ultra-fast electron diffraction imaging can reveal that information. Now, a group of researchers from the U.S. Department of Energy's (DOE) Brookhaven National Laboratory have developed a new and improved version of electron diffraction at Brookhaven's Accelerator Test Facility (ATF)—a DOE Office of Science User Facility that offers advanced and unique experimental instrumentation for studying particle acceleration to researchers from all around the world. The

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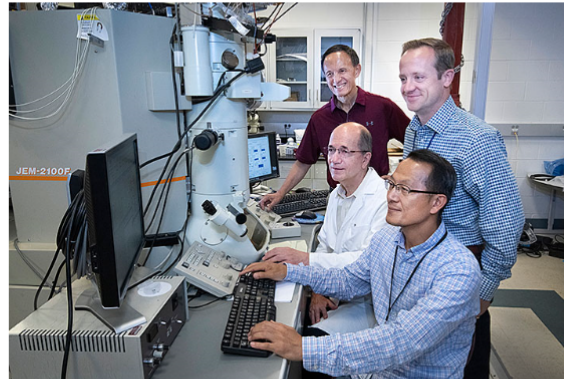
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Measuring the Charge of Electrons in a High-Temp Superconductor

Scientists found a large concentration of electron pairs outside key temperature and energy ranges; this finding could inform the search for new materials that conduct electricity without resistance at unusually high temperatures

August 21, 2019



[+ ENLARGE](#)

Brookhaven Lab scientists Myung-Geun Han (sitting front), Ivan Bozovic (sitting back), Yimei Zhu (standing back), and Anthony Bollinger of the Condensed Matter Physics and Materials Science Division built electronic transport devices that sandwich a thin layer of an insulating material in between two thicker layers of superconducting materials. They characterized these devices using an electron microscope (seen in background). In collaboration with scientists at Rice University and the University of Connecticut, the team discovered that a high percentage of electron pairs—which are known to carry superconducting current—exists well above expected temperature and energy ranges in a material that conducts electricity without energy loss at unusually high temperatures.

bnl.gov/newsroom/news.php?a=215562

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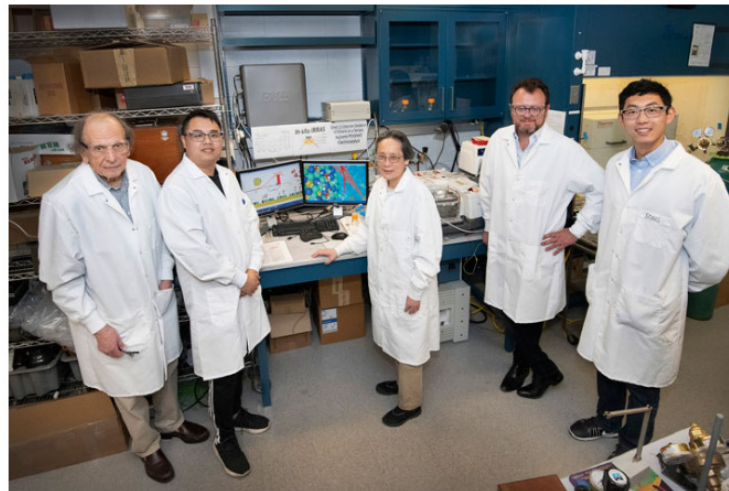
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New Core-Shell Catalyst for Ethanol Fuel Cells

Greatly boosts efficiency of ethanol electro-oxidation, offering promise for liquid-fuel-cell-powered drones

June 7, 2019



Brookhaven Lab members of the research team that developed and characterized a new core-shell catalyst

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Brookhaven National Laboratory

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Direct 12-Electron Oxidation of Ethanol on a Ternary Au(core)-PtIr(Shell) Electrocatalyst

Zhixiu Liang, Liang Song, Shiqing Deng, Yimei Zhu, Eli Stavitski, Radoslav R. Adzic, Jingyi Chen* and Jia X. Wang*

Cite this: *J. Am. Chem. Soc.* 2019, 141, 24, 9629–9636Publication Date: May 26, 2019
<https://doi.org/10.1021/jacs.9b03474>

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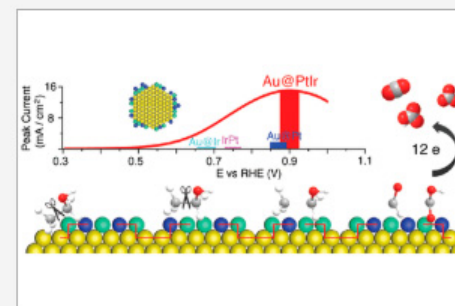
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Abstract

Understanding the roles of metals and atomic structures in activating various elementary steps of electrocatalytic reactions can help rational design of binary or ternary catalysts for promoting activity toward desirable products via favorable pathways. Here we report on a newly developed ternary Au@PtIr core–shell catalyst for ethanol oxidation reaction (EOR) in alkaline solutions, which exhibits an activity enhancement of 6 orders of magnitude compared to AuPtIr alloy catalysts. Analysis of in situ infrared reflection absorption spectra for Au@PtIr and its bimetallic subsets, Au@Pt and PtIr alloy, found that monatomic steps and Au-induced tensile strain on PtIr facilitate C–C bond splitting via ethanol dissociative adsorption and Ir promotes dehydrogenation at low potentials. As evidenced by the CO band being observed only for the PtIr alloy that is rather inactive for ethanol dissociative adsorption, we propose that splitting the C–C bond at the earliest stage of EOR activates a direct 12-electron full oxidation pathway because hydrogen-rich fragments can be fully oxidized without CO as a poisoning intermediate. The resulting synergy of complementary effects of Au core and surface Ir leads to an outstanding performance of Au@PtIr for EOR as characterized by a low onset potential of 0.3 V and 8.3 A mg^{−1}_{all-metals} peak current with 57% currents generated via full ethanol oxidation.



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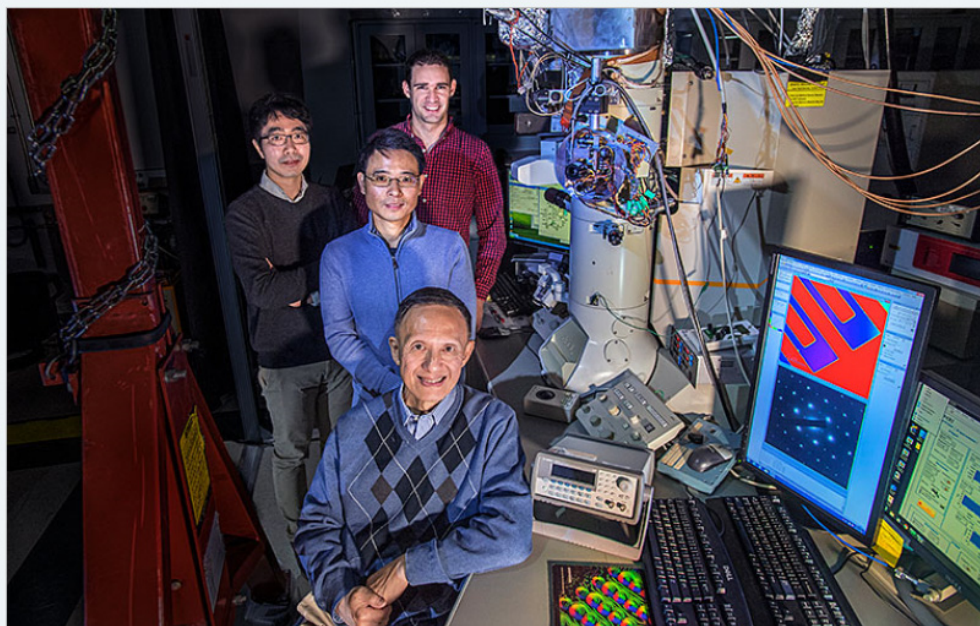
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Electron Pulsed Source Wins 2019 R&D 100 Award

Brookhaven and its collaborators developed a laser-free device for probing fast atomic-scale processes in energy and bio materials. [More...](#)



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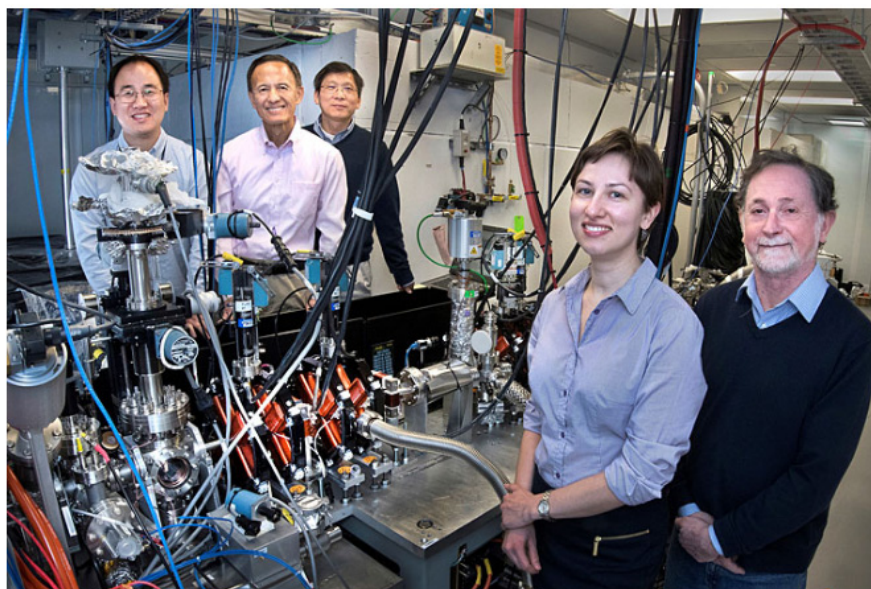
Contact: [Peter Genzer](#), (631) 344-3174 | Written by Justin Eure

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Scientists Pinpoint Energy Flowing Through Vibrations in Superconducting Crystals

Interactions between electrons and the atomic structure of high-temperature superconductors impacted by elusive and powerful vibrations

April 27, 2018



The Brookhaven/Stony Brook team (from left): Junjie Li, Yimei Zhu, Lijun Wu, Tatiana Konstantinova, and Peter Johnson.

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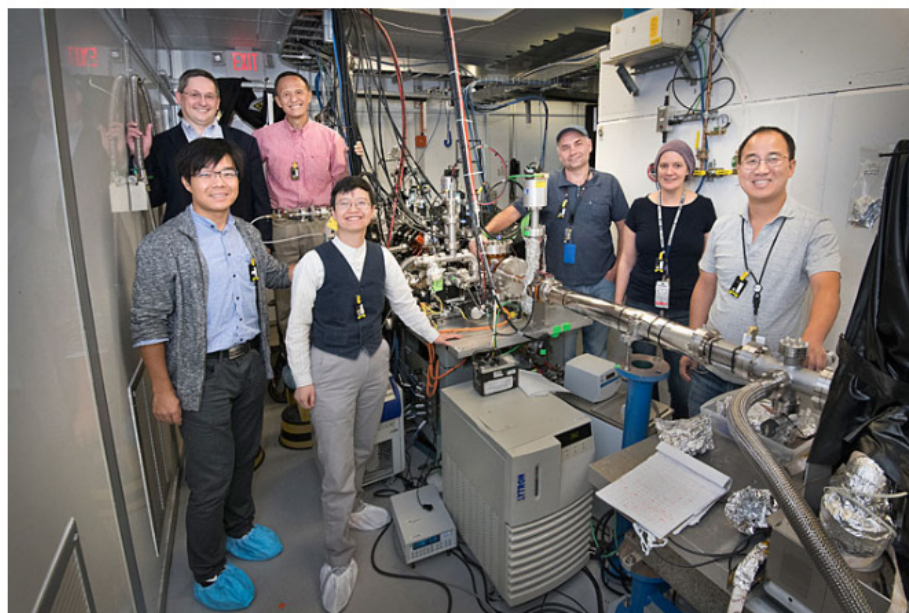
By [Ariana Tantillo](#)

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Making a Movie of Nanocrystals' Structural Evolution

Combined ultrafast snapshots suggest that the crystal symmetry of copper sulfide nanocrystals changes due to interactions between electrons and atoms vibrating in the crystal lattice—an understanding of which could help scientists optimize the functionality of superconductors, magnetic materials, and other strongly correlated systems

October 4, 2018



(Clockwise from left) Jun Li, Mark Palmer, Yimei Zhu, Jing Tao, Mikhail Fedurin, Christina Swinson, and Junjie Li with the new ultrafast electron diffraction instrument installed at Brookhaven Lab. The team used this instrument to make an atomic-scale "movie" capturing the dynamic structural changes of copper sulfide nanocrystals. [+ ENLARGE](#)



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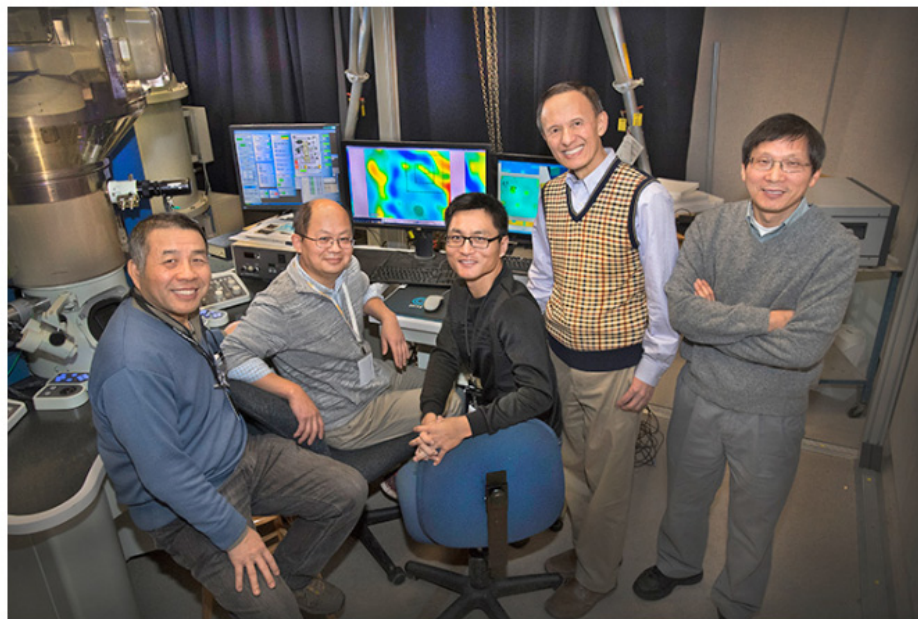
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Surprising Discovery Could Lead to Better Batteries

Scientists have observed how lithium moves inside individual nanoparticles that make up batteries. The finding could help companies develop batteries that charge faster and last longer.

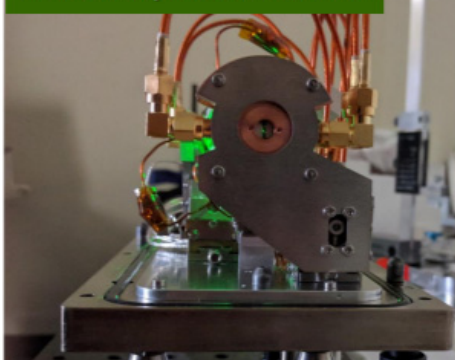
January 12, 2018



Brookhaven scientists are shown at the Condensed Matter Physics and Materials Science Department's TEM [+ENLARGE](#) facility, where part of the study was conducted. Pictured from left to right are Jianming Bai, Feng Wang, Wei Zhang, Yimei Zhu, and Lijun Wu.



DOE SBIR/STTR Success



Electron beam modulating apparatus for producing a high-frequency, pulsed electron source for time-resolved commercial transmission electron microscopes. Device viewed from the top during the laser alignment procedure. The unit consists of a beam focusing element and a GHz buncher. All components are mounted on a vacuum compatible 3-axis translation stage

EUCLID TECHLABS

Sometimes the most notable innovations in science come from linking traditionally separate or independent knowledge. Specifically, synergies happen when mechanisms known and adopted in one scientific domain are modified to produce new concepts in a different domain. Often, such cross cutting approaches need to be encouraged because of the highly specialized fashion in which each scientific field evolves. Yet, sometimes they spur spontaneously as the result of a fortuitous encounter. Euclid TechLabs LLC (Euclid for short) is an R&D small business specializing in the design and development of particle accelerators and their components for high energy and nuclear physics applications.

FACTS

PHASE III SUCCESS

Euclid's product sales have reached \$ 1.6 M in 2016-2017. Phase III achievements include a \$680k contract from NIST in collaboration with BNL and JEOL

IMPACT

Euclid's electromagnetic-mechanical buncher makes it possible for an electron microscope to reach the ultimate space-time resolution of 10^{-20} to 10^{-23} m-s necessary to probe ionic, charge, and spin transport in advanced energy materials.

DOE PROGRAMS

Nuclear Physics (NP), Basic Energy Sciences (BES), High Energy Physics (HEP).

This is news for DOE SBIR on the pulse device we developed for ultrafast electron microscopy, in collaboration with a small company Euclid TechLabs.

We have received three SBIRs. The news release was issued in March 2018.