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MPA MaterialsMatter

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Vivien Zapf

A force unleashed

By Kirsten Fox
Communication Arts and Services (IRM-CAS)

During the last year, while Vivien Zapf was researching magnetoelectric effects and Bose-Einstein condensation in quantum magnets she accomplished a few other things: presenting five talks, publishing 10 journal articles, participating on six committees and funding panels, mentoring a postdoctoral researcher and student, writing most of a science fiction book, and acting as a publicity liaison for her group. And one more thing: raising her daughter, Anya.

In the Los Alamos land of overachievers, one might say Zapf has, well, surpassed expectations. She admitted delegating work is a challenge.

"You want to do everything yourself, but ultimately, your research is limited as opposed to working with other people," she said.

Credit: Robb Kramer, ADEPS

Zapf, a technical staff member at the National High Magnetic Field Laboratory's Pulsed Field Facility (MPA-NHMFL) at Los Alamos National Laboratory, studies magnetic field-induced electric polarization in organic magnets. The magnet lab's ultra-fast magnetic field pulses allow her team to perform sensitive measurements of the electric polarization and demonstrate the coupling of the electric state to the magnetic order that allows reversal of the electric polarization direction. Quantum magnets containing copper ions could open doors to many new applications including new types of hard drives, microwave devices, photonics, resonators, transistors, and transducers.

To circumvent roadblocks to creating this rare type of magnetic system, Zapf looks for compounds with long-range order, which she says can lead to significant magnetoelectric couplings. Organic

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Los Alamos National Laboratory

From David's desk

Laboratory Directed Research and Development (LDRD) plays an important role in MPA Division. Clearly this is true from a financial perspective. In fiscal year 2008, LDRD accounted for 28% of funding for the Division. This year, LDRD accounts for 33% of the current Division funding. From a technical perspective, LDRD is enabling us to pursue new directions ranging from developing novel scintillators to creating genetically engineered polymer libraries and from demonstrating terahertz photonic devices to exploring the effects of spin in organic electronic materials. Some LDRD projects are already paying off in terms of providing a basis for new programmatic efforts. Others are paying off through enhancing the reputation of MPA personnel through high-profile publications and opportunities to present their research at international conferences. Still others provide the basis for collaborations both within the Laboratory and externally. As we approach the next opportunity to compete for LDRD, it is worth reflecting on the benefits we can derive from LDRD, as well as considering how we might focus our technical efforts to the best advantage of the Division.

The success of the Division in LDRD is a testament to the quality of our personnel and their innovative ideas. The competition for LDRD funding has been substantial, with typically only one in 10 proposals obtaining funding. Across the Laboratory, LDRD accounts for about 7% of total funding. At four times that value, MPA is among the top divisions at Los Alamos for LDRD funding. The ultimate goal of the LDRD program, as defined by Congress, is to enhance the scientific vitality of the Laboratory. The strong success rate of MPA in the LDRD competition carries with it an obligation to accomplish this mission. In an era when we can expect the budget of the Laboratory's core mission area to decline, a key element of scientific vitality is establishing new programmatic directions that enable us to diversify our funding base. The substantial funding the Division currently enjoys in LDRD provides both an opportunity and an obligation to seek external follow-on funding.

MPA is a division of entrepreneurs. The innovative concepts that are proven through LDRD investment, and the new capabilities we create through LDRD research should form the basis for proposals to external sponsors. We must work together, across groups, at all levels of MPA management, and with our program managers, towards this goal. While LDRD can continue to provide us with unique opportunities to explore new ideas and create new capabilities, our ultimate goal should be to draw new programmatic funding that is shared across the Laboratory and that justifies the balance between LDRD funding and external funding within MPA Division.

As we look to the future, it is important to ask how Division management should influence LDRD proposals. I remain a strong believer in the concept of grass-roots innovation as a core principle underlying good science. However, management can set a framework for the scientific and technical directions for LDRD proposals. In MPA Division, we are particularly interested in LDRD concepts that would enable us to compete effectively in areas of emerging national needs. Reducing global threats and meeting the nation's energy needs both provide significant technical challenges for MPA staff to pursue. These areas will also provide good opportunities for expanding our programmatic funding. We have tried to set the stage for these areas by influencing the technical strategies within the LDRD grand challenges for Directed Research. (See current MPA LDRD DR projects on the next page.) As we proceed through LDRD DR endorsements, we will stress strong science, integrated efforts engaging other divisions, new ideas that take us beyond our existing LDRD DR project portfolio, and opportunities to seed new capabilities for program development.

Finally, I would like to comment briefly from my perspective as the former LDRD program manager on what makes a compelling LDRD DR proposal. Innovative ideas and good science are clearly critical elements, but ideas with inherently obvious connections to the Laboratory's unique capabilities fair best. In addition, it is essential to build a strong and integrated research team; a team where the role of each individual is clear and essential to success. Also, while fulfilling all goals of the proposal should be a stretch, significant progress towards the goals should be realistic. "Fratricide," where competing proposals on similar research topics vie unsuccessfully for funding, is a real problem and is best resolved before proposal submission. To prepare a proposal that meets these criteria takes substantial effort, planning, and a significant investment of time.

David Watkins, MPA Deputy Division Leader

Current LDRD projects with significant MPA involvement

The following is a list of LDRD DR projects with substantial MPA involvement. Projects initiated in 2006 and 2007 will end this fiscal year.

20060043DR	Strongly Correlated Electrons: Duality and Implications	Cristian Batista
20070013DR	Correlations and Control of Properties of Metallic U and Pu	Jeremy Mitchell
20070060DR	Metamaterials for Threat Reduction Applications: Imaging, Signal Processing, and Cloaking	Antoinette Taylor
20070064DR	Coexistence of Magnetic and Superconducting Electrons in Strongly Correlated Matter	Joe Thompson
20070077DR	Quantum Control in Condensed Media for Studies of Direct Optical Initiation of Explosives	David Moore
20070096DR	Biomimetic Hydrogen Production by Photoinitiated Transition Metal Catalysis	Richard Dyer
20070505DR	Multiscale Modeling of Strongly Interacting Systems	Robert Ecke
20080015DR	Hot Spot Physics and Chemistry in Energetic Materials Initiation	Dana Dattelbaum
20080037DR	Design, Synthesis, and Theory of Molecular Scintillators	Rico Del Sesto
20080057DR	Carrier Multiplication in Nanoscale Semiconductors for High-Efficiency, Generation-III Photovoltaics	Victor Klimov
20080085DR	Construction and Use of Superluminal Emission Technology Demonstrators with Applications in Radar, Astrophysics, and Secure Communications	John Singleton
20080097DR	Ultrafast Nanoscale XUV Photoelectron Spectroscopy	George Rodriguez
20090017DR	Predictive Design of Noble Metal Nanoclusters	Jennifer Martinez
20090022DR	Understanding Anisotropy to Develop Superconductors by Design	Filip Ronning
20090061DR	Enhance Radiation Damage Resistance via Manipulation of the Properties of Nanoscale Materials	Michael Nastasi

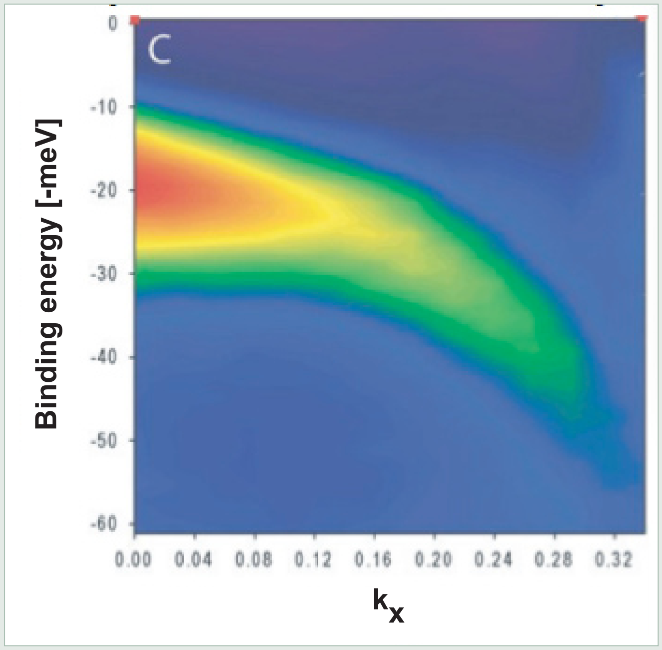
New hydrogen storage project funded: Part of new Hydrogen Storage Engineering Center of Excellence

Troy Semelsberger (MPA-MC) is the Los Alamos principal investigator of a newly funded hydrogen storage project. This new project, which is funded by the Department of Energy's (DOE) Energy Efficiency and Renewable Energy (EERE) Office of the Hydrogen, Fuel Cells and Infrastructure Technologies Program, is part of the new Hydrogen Storage Engineering Center of Excellence. Partners in this center include Pacific Northwest National Laboratory, National Renewable Energy Laboratory (NREL), United Technologies, the Jet Propulsion Laboratory, General Motors, Ford, Lincoln Composites, and the University of Oregon. Savannah River National Laboratory leads the center for DOE. The engineering center will be funded at about $6 million in FY09, and is expected to run for five years with a total project cost of more than $40 million.

This team of researchers will address the significant engineering challenges associated with developing low-pressure, materials-based hydrogen storage systems that will enable fuel cell vehicles to meet customer expectations for driving range and performance. These projects will be incorporated into the DOE's National Hydrogen Storage Project, which currently focuses on hydrogen storage materials development. Los Alamos National Laboratory (LANL) leads the Chemical Hydrogen Storage Center of Excellence for DOE. This new engineering center will work closely with the LANL center as well as the Metal Hydride and Sorption Centers led by Sandia National Laboratory-Livermore and NREL, respectively.

This team of researchers will address the significant engineering challenges associated with developing low-pressure, materials-based hydrogen storage systems that will enable fuel cell vehicles to meet customer expectations for driving range and performance.

First experimental observation of a kink in the dispersion of *f*-electrons



◄ *Expanded view of the quasiparticle band A dispersing from the zone center, with a clearly visible kink in the middle part of the panel.*

Strong interactions in correlated electron systems may result in the formation of heavy quasi-particles that exhibit kinks in their dispersion relation. However, kinks in band dispersions have so far been observed in *d*–electron systems, but not in f-electron systems. Los Alamos researchers and collaborators have made the first experimental observation of a kink structure in *f*-electron systems. The scientists discovered a kink energy scale of 21meV and an ultra-small intrinsic peak width of 3 meV in an *f*-electron material, USb_2 (figure above). This new finding extends the context of quasiparticle band renormalization from *d*-electrons to *f*-electrons, creating a link between high temperature superconductors and heavy fermions and actinides.

The researchers propose a new model of point-like Fermi surface renormalization to explain the spectroscopic properties of the kink. Spectral weight is incoherently shifted away from the Fermi energy, but Luttinger's theorem requires the Fermi volume to remain constant. Although the renormalized quasiparticle band in USb_2 starts at 17 meV below the Fermi energy, the spectrum associated with this band still shows properties of a renormalized Fermi liquid, such as the kink in the dispersion relation and ultra-sharp quasiparticle peaks. The scientists assign these features to interband electron-boson scattering processes, with asymmetry being controlled by intraband scattering.

The research was published: "Observation of a Kink in the Dispersion of *f*-electrons," by Tomasz Durakiewicz, John Joyce, Eric Bauer, and Kevin Graham (MPA-10); John Sarrao (SPO-SC); David Moore (MST-16); P. Riseborough (Temple University) ; C. G. Olson (Ames Laboratory); P. M. Oppeneer, S. Elgazzar (Uppsala University); E. Guziewicz (Polish Academy of Sciences); and M. T. Butterfield (Lawrence Livermore National Laboratory), appears in *Europhysics Letters 84*, 37003 (2008). The work was performed under the auspices of the DOE and the LANL LDRD Program.

Technical contact: Tomasz Durakiewicz

Eric Brosha elected to office in the Electrochemical Society

▲ *Eric Brosha (MPA-11)*

Eric Brosha (MPA-11) was elected as the secretary/treasurer of the Sensor Division at the 214th meeting of the Electrochemical Society. The meeting, held in Honolulu, HI, was also the Pacific Rim Meeting on Electrochemical and Solid-state Science. Brosha's duties will include maintaining records of division meetings and related correspondence in addition to overseeing sensor division finances.

Brosha's research interests include the development of electrochemical gas sensors, synthesis and study of fuel cell catalysts, the study of impurity effects on polymer fuel cells and components, x-ray diffraction, x-ray fluorescence spectroscopy, and thermal analysis of materials. He received seven U.S. patents for the development of new types of electrochemical gas sensors. In 1999, one of his inventions was selected by *R&D Magazine* as one of the 100 most significant research and development contributions to U.S. industry and technology.

When materials are tuned to a critical point at absolute zero temperature, quantum effects dictate universal behavior in material properties. The presence of a singular point, depicted as the black hole, is revealed through its unusual electronic properties that make the superconducting material behave simultaneously as a nonmagnetic material and a magnetic material. Credit: Tuson Park (MPA-10)

New mechanism for superconductivity described

Los Alamos researchers have developed an explanation for superconductivity that may open the door to the discovery of new, unconventional forms of superconductivity. In a recent *Nature* letter, research led by Tuson Park and Joe D. Thompson (both in MPA-10) describes a new explanation for superconductivity in non-traditional materials—one that describes a potentially new state of matter in which the superconducting material behaves simultaneously as a nonmagnetic material and a magnetic material.

Superconducting materials carry a current without resistance, usually when cooled to temperatures nearing the liquid point of helium (nearly 452 degrees below zero Fahrenheit). Superconductors hold promise for carrying electricity from one place to another without current loss and providing indefinite electric storage capacity. However, the cost of cooling materials to the required extremely low temperatures currently limits the practicality of superconductors. If superconductors could be designed to operate at temperatures closer to room temperature, they could become more practical.

Traditional theories of superconductivity hold that electrons within certain nonmagnetic materials can pair up when jostled together by atomic vibrations known as phonons. Thus the phonons provide the "glue" that makes superconductivity possible.

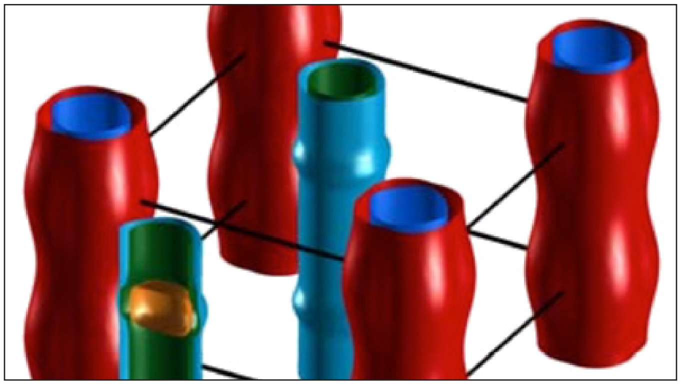
Los Alamos researchers now describe a different type of "glue" giving rise to superconducting behavior. When they cooled a material of cerium, rhodium, and indium to just above absolute zero, nearly minus 459 degrees Fahrenheit; the material exhibited superconducting behavior. Then they subjected the material to pressure changes and a magnetic field to perturb the alignment of electrons within the material. This treatment induced very high quantum fluctuations in the material, making it difficult for the electrons to move. This electronic "traffic jam" should discourage electron pairing by phonons; nevertheless, the material continued to exhibit superconducting behavior.

Based on the material's behavior under different pressures, temperatures, and magnetic fields; the researchers believe that the material reaches a quantum critical point near absolute zero. At this quantum critical point, the material retains properties of a metal with highly ordered electrons and highly disordered ones—a previously undescribed state of matter. The scientists believe that this quantum critical point provides a mechanism to pair electrons into a quantum state that gives rise to superconducting behavior. The research helps explain a mechanism for superconductivity without phonons. The quantum critical point could be analogous to a black hole, in which superconductivity is observed (figure above), but researchers cannot see inside to understand why. Formation of superconductivity in the vicinity of a singular critical point defies the conventional belief that turbulent electronic fluctuations are not beneficial to form the macroscopic quantum state.

A new mechanism for the electron-pairing glue that gives rise to superconductivity could allow researchers to design new materials that exhibit superconducting materials at higher temperatures. In addition to Park and Thompson, researchers include: Vladimir Sidorov, Filip Ronning, Han-Oh Lee, Eric Bauer, Roman Movshovich, and Yoshifumi Tokiwa (all of MPA-10); John Sarrao (SPO-SC); and Jian-Xin Zhu (T-4). Reference: "Isotropic Quantum Scattering and Unconventional Superconductivity," *Nature* **456**, 366-368 (2008). DOE's Office of Science and LANL LDRD funded the research.

— By James E. Rickman, CGA-CO

The Fermi surface of LaFePO. The concentric red and dark blue cylinders correspond to electron bands; the turquoise and green cylinders and gold spheroids correspond to hole bands.



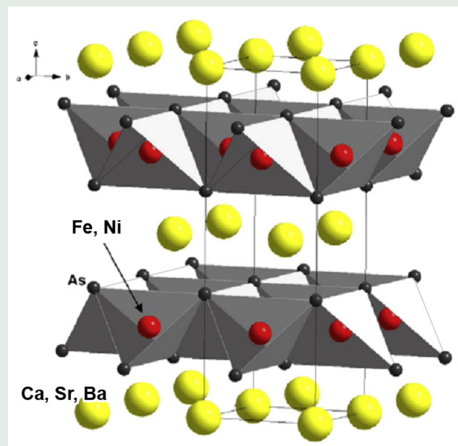
New iron-based superconductor studied

Ross McDonald (MPA-NHMFL), and collaborators from the University of Bristol, United Kingdom and Stanford University, measured quantum oscillations in the material LaFePO, the first of a new class of recently discovered iron-based superconductors. Quantum oscillations provide a bulk probe of the electronic structure, giving detailed information about the Fermi surface topology and mass renormalization. The Fermi surface is the surface of constant energy in momentum space that separates occupied and unoccupied electron states. The tetragonal layered structure of LaFePO is made of alternating highly conductive FeP layers and poorly conducting LaO layers stacked along the c axis; therefore the Fermi surface is expected to be quasi two-dimensional. The scientists used low temperature torque magnetometry and transport in high static magnetic fields (45 T) for the measurements.

The researchers determined that the Fermi surface of LaFePO is composed of quasi two-dimensional nearly-nested electron and hole pockets with moderate enhancement of the quasiparticle masses (see figure above). The near-perfect matching between the hole and the electron orbits suggests that LaFePO may be close to a spin/charge density wave transition and that magnetic fluctuations are an important ingredient in the physics of the iron-based superconductors. The work is an important step in understanding the novel mechanisms of superconductors. Reference: A.I. Coldea, J.D. Fletcher, A. Carrington, J.G. Analytis, A.F. Bangura, J.-H. Chu, A.S. Erickson, I.R.Fisher, N.E. Hussey, and R. D. McDonald, "Fermi Surface of Superconducting LaFePO Determined from Quantum Oscillations," *Physical Review Letters* **101**, 216402 (2008). The National High Magnetic Field Laboratory user program supported the LANL work.

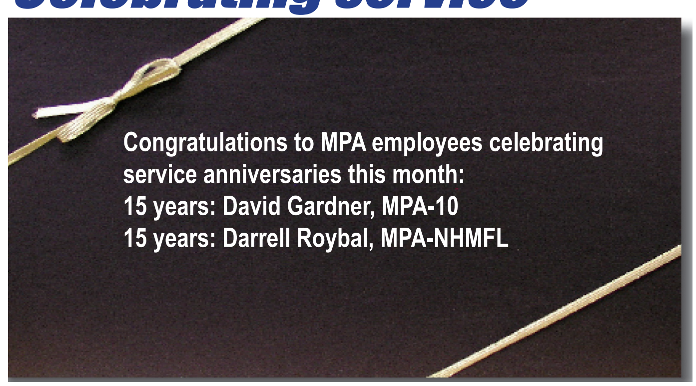
Research on three new superconductors presented at international workshop

Filip Ronning (MPA-10) represented MPA Division at the International Workshop on Iron (nickel)-Based Superconductors, held in Beijing, China. He presented an invited talk, "Superconductivity in Barium Nickel Arsenide and Calcium Iron Arsenide." Ronning's presentation described research in collaboration with Eric Bauer, Tuson Park, Nobuyuki Kurita, Han-Oh Lee, Tomasz Klimczuk, Seung-Ho Baek, Roman Movshovich, and Joe Thompson (all in MPA-10); Brian Scott (MPA-MC); and Heather Volz (MST-6). The scientists discovered three new superconductors with transition temperatures up to 13 degrees Kelvin. This discovery adds to the variety of compounds known to be superconductors in this materials class. Ronning described the physical properties of these materials, how the team made the discovery, and the correlation of physical properties with the superconducting transition temperature. Ronning also presented MPA-10's work on iron-based superconductors and strongly correlated materials at the Institute of Physics and Applied Physics at the Yonsei University in Seoul, Korea.



The crystal structure in which the team found superconductivity for $CaFe_2As_2$ (at 13K under pressure), $BaNi_2As_2$, and $SrNi_2As_2$.

Celebrating service



Zapf profile. . . *continued from page 1*

quantum magnets have strongly polarized chemical bonds and their soft structure allows magnetic forces to create significant strains in the lattice. In the new class of compounds Zapf uses, the bare crystal structure has inversion symmetry, but it is broken by the long-range order of the magnetic spins. A unique axis is created, allowing a close coupling between magnetic and electric effects.

Drawn by the world's most powerful magnets

Scientists at the Los Alamos magnet lab achieved two world records with the 100 Tesla Multi-shot Magnet, which produces the highest non-destructive field in the world. A tesla denotes magnetic strength, and the Earth's magnetic field is one twenty thousandth of a tesla. Scientists worldwide use this magnet for a variety of research that provides precise measurements, including how materials behave under the influence of high magnetic fields or to research phase transitions—from superconductors to nanotechnology. A high magnetic field can act as a probe of the way electrons behave in a material as well as be used to create new phases of matter.

The lab's powerful pulsed magnets range from 50 tesla shots that are 300 milliseconds long to a two-second long pulsed magnet. Most magnets at the lab process around 60 tesla shots—"a Snickers bar worth of energy pulsed in milliseconds," said Zapf—and the magnets succumb to stress and fail, most after 600 tests. The 100 T Multi-shot Magnet can be used multiple times per day.

The magnet lab also developed the "biggest and smallest magnet," according to Zapf, about as large as a human thumb, designed to reach 240 tesla for 10 microseconds. This magnet utilizes inexpensive materials for the coil (unlike some multi-shot magnets that use platinum) and is repaired after every shot. It can be used with optical techniques and provides answers to physicists about phase transitions at high magnetic fields.

"Our main interest is doing the experiment, not beating a record," said Charles Mielke, NHMFL-PFF user program director. "This magnet's force is over a million pounds per square inch. It puts holes in half-inch thick steel, but does not damage the sample's half millimeter thick fiberglass tube. Amazing."

The Pulsed Field Facility is one of three campuses of the National High Magnetic Field Laboratory, which has facilities at Florida State University and the University of Florida.

Living life to the fullest

Zapf, raised by nomadic parents, graduated from Harvey Mudd College and the University of California, San Diego, where she received her doctorate in 2003. She and her 10-month-old daughter live in White Rock with her husband who flies in from the West Coast on weekends.

When asked about her hobbies, the busy mother and scientist joked, "What did I use to like to do?" The avid gardener knew when her daughter was born there would be little time for leisure and she tore out all her roses.

A few years ago Zapf completed most of a young adult fantasy fiction volume. It has a female protagonist battling to survive on a planet torn between two ecologies that cannot survive together—a "Romeo and Juliet of clashing cultures," she said—paralleling her research with opposite poles or, perhaps signifying Zapf's competing and demanding responsibilities.

She attacks her ambitions with verve. "I don't know where it is going, but it can take off in any direction," said Zapf, discussing her goal of finding new organic magnetoelectric compounds, which have ties with energy research. "It could open a whole new field of devices. It'll be big—it's exciting."

International cell phone available

Most American cell phones are not compatible with the cellular service in other countries. MPA-DO has purchased an international cell phone that is available for temporary use by travelers on official Laboratory business outside the United States. Contact Susie Duran (susiew@lanl.gov, 5-1131) to reserve.

Timely travel expense report submittal

Travelers must file an expense report within 15 days of the trip. Division chiefs of staff and executive administrators receive monthly reports listing trips lacking expense reports. Authorization requests (AR) lacking an expense report filed within 45 days from trip will be closed, requiring an AR request to be approved.

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