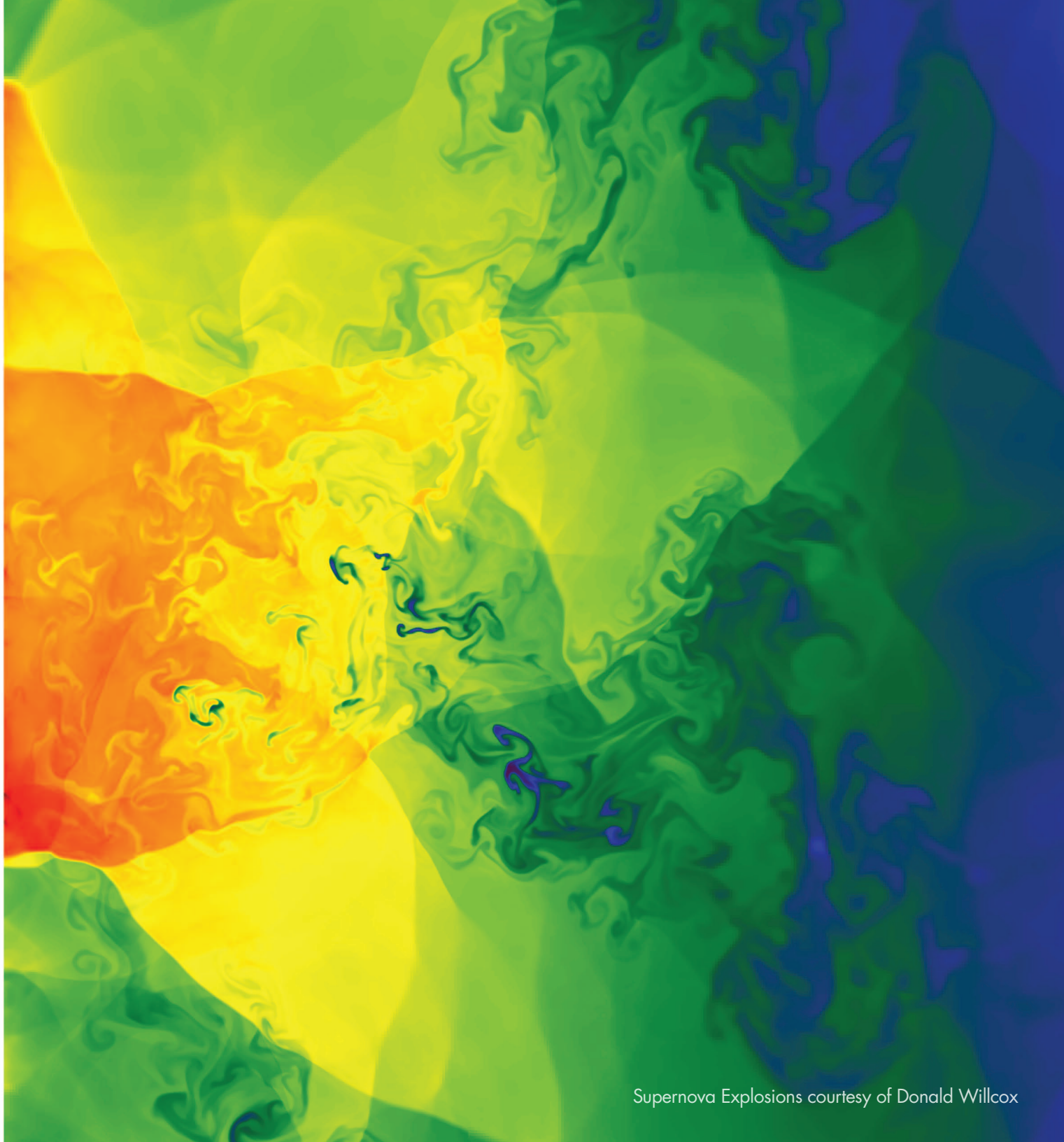
iACS
INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

ANNUAL REPORT 2013



Supernova Explosions courtesy of Donald Willcox

MESSAGE FROM THE DIRECTOR

IACS Director Robert Harrison

Dear Friends and Colleagues,

It has been a fast and energetic first year for The Institute for Advanced Computational Science (IACS), and in this brief message, in addition to talking about our activities and plans, I hope to convey to you our huge excitement and sense of opportunity.

Nicely capturing our multidisciplinary vision, our first IACS proposal was a collaboration between sociology, computational science, and economics that aimed to empower the National Science Foundation (NSF) computing community through the provisioning of resources in the cloud and by changing the dynamics of user engagement to a collaborative and collective approach. A successful proposal to the NY State Empire Innovation Program brought $1M to support senior faculty startup at SBU.

Little would have been possible without the commitment and strong support of both the university leadership and the donors of our endowment. The vision and energy of Provost Dennis Assanis and Associate Vice Provost Peter Paul were instrumental to our foundation and remain so to our future success, and they with President Samuel Stanley have committed time and resources to ensure our growth. We owe them and their teams a huge debt of thanks, along with the leadership and staff of the Stony Brook Foundation including Dexter Bailey and Jason Hsueh. Deputy Provost Brent Lindquist, the former head of the Applied Mathematics and Statistics department, has also been a strong advocate of IACS and computational science in general, an example of which is his successful proposal to the Long Island Empire State Development grant for a $1M high-performance cluster. The baton was passed to us by Professor James Glimm who led the preceding Stony Brook Computational Science Center, and whose energy and deep experience still serve as a foundation for computational science across all of Stony Brook. At Brookhaven National Laboratory (BNL), we would like to thank Dr. Reinhold Mann, the Associate Laboratory Director for Environmental, Biological and Computational Sciences, and the staff of the Computational Science Center.

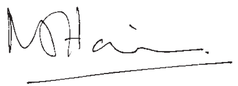
Our generous endowment, $10M from an anonymous donor matched by $10M from the Simons Foundation, is truly transformational and will help enable many of our aspirations. We are very grateful for this support. I would like to direct you to page 11 where you will see the significant impact these donation are having on our research.

As I write this text, I have on my laptop about 150 applications for our first round of new faculty hires: two senior and two junior positions in Computer Science and Applied Mathematics and Statistics. The applicants include some very talented and accomplished people who share our sense of potential for IACS, SBU, and SUNY. Our vision is that these new members will establish research collaborative programs that cut across our institute and Stony Brook University, and address some of the fundamental challenges in “how we compute.” Of particular concern to me is making progress on reducing the overwhelming complexity of computation that slows innovation and creates a huge entry barrier for individuals and even entire disciplines that are new to computation. This complexity is increasing as we strive to solve bigger problems and exploit new computer technologies, and multiple government agencies are now investing in approaches to what the NSF refers to as sustainable software, which really includes all aspects of computation - not just raw lines of code. Our hiring is coordinated with BNL, and we envision multiple joint appointments that will also parlay the eight new faculty lines committed to IACS into perhaps ten or more new researchers.

In the body of this, our first annual report, you can read about some of our research highlights and accomplishments, learn about our construction plans and first major computer purchase, and see our current faculty, students and staff.

Finally, we at IACS recognize the truly transformational contributions of Lynn Allopenna, our administrative director who joined us in March 2013 from her previous role as director of the SBU postdoctoral program. Lynn’s energy, insight, experience, and professionalism have made IACS real – thank you!

Yours sincerely,



MISSION STATEMENT

Cutting edge and collaborative, bridging frontiers between disciplines, the Institute for Advanced Computational Science (IACS) is a powerful incubator generating ideas that will influence not only SBU but the state, the nation and our international research communities. IACS seeks to make sustained advances in the fundamental techniques of computation and in high-impact applications including engineering and the physical, life, and social sciences. We are led by a community of inclusive, forward-thinking and world-renowned researchers working in a highly collaborative environment with access to a wide range of resources.

Because of the pervasive entrepreneurial, think-tank culture of support and encouragement at IACS, our students make connections that elevate their careers and electrify their curiosity. We seek active, interdisciplinary thinkers who take intellectual risks and find excitement in developing and sharing ideas and technologies on a global stage – concepts that will affect our world, from predicting sustainable sources of green energy to harnessing the power of big data in an effort to understand and control the world around us. Here, a day might begin with a conversation between a chemist and an applied mathematician, and end with plotting a new project with a social scientist and a computational linguist. The common threads are the inherent multidisciplinary nature of modern science, how we compute, and the technology that drives many advances in our fields. Against this backdrop, the IACS plays a lead role in connecting science and its people within the academic community and reaching out to help local industries by increasing their ability to adopt the tools of modern simulation and truly effect a change in the world.

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William Scott Thornton Research Associate Professor

After receiving his BS in Electrical Engineering from Auburn University, Dr. Thornton worked as an application engineer for Asea Brown Boveri (ABB) for the pulp and paper industry. Later, he went to work as a software developer for Northrop Grumman at the Air Force Wargaming Institute (AFWI). After 6 years of working as a software developer, Dr. Thornton pursued and received his PhD in Physics under the direction of Adolfo Eguiluz and Robert Harrison at the University of Tennessee where he focused on complex oxides and numerical techniques in density functional theory. His research is concerned primarily with the implementation of density functional theory and other electronic structure methods for crystalline systems using multiresolution analysis techniques. He is a lead developer for the software MADNESS (Multiresolution ADaptive Numerical Environment for Scientific Simulation). He also has an interest in many-body methods such as GWA, DMFT, coupled-cluster, CI, etc.

Predrag Krstic Research Professor

Dr. Predrag Krstic is a Research Professor at the Institute for Advanced Computational Science, a senior staff scientist at the Joint Institute for Computational Sciences, an adjunct professor in the Department of Physics and Astronomy at the University of Tennessee, and founder and owner of the TheoretiK consulting. He has worked in the Physics Division at Oak Ridge National Laboratory in the Theoretical Atomic Physics program since 1995, where he retired as a member of the senior research and development staff and project manager. He obtained his Ph.D. at CC of CUNY in 1981 on the theory of multiphoton processes, and he received his BSC and MSC in technical physics and technical plasma physics from the University of Belgrade. His research covers a wide range of fields in theoretical atomic physics, plasma physics and nuclear fusion, computational physics and chemistry, plasma-surface interactions, molecular electronics and bionanotechnology. His work has been disseminated in more than 200 papers in peer-reviewed journals, in several patents, in more than 80 talks at scientific conferences and seminars, and in a number of international atomic databases. He is a contributor to book chapters; an editor of a number of conference proceedings; a PI and Co-PI on many grants with DOE, NIH, NSF, and IAEA; a consultant for the International Atomic Energy Agency; a Fellow of the American Physical Society; and an organizer and co-organizer for various international conferences.

Lynn Allopenna

Lynn Allopenna was hired in March of 2013 as the Administrative Director for the Institute for Advanced Computational Science. She has worked at Stony Brook University for eight years. Her position for the previous two years was as Assistant Dean for Postdoctoral Affairs, where she created the office and was the sole administrator since the office's inception in Fall 2010. Before becoming Assistant Dean, Lynn worked as the Assistant to the Chair in the Materials Science & Engineering Department. Prior to her initial hire at SBU Lynn worked as an executive editor at Times Beacon Record Newspapers and as an administrator at Crown Publishing as well as at Bank Street College of Education in Manhattan.

1 Philip B. Allen
Professor
Physics & Astronomy
Stony Brook University

2 Patricia Kovatch
Associate Dean for
Scientific Computing
Mount Sinai School
of Medicine

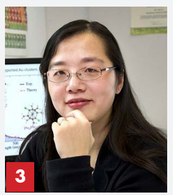
3 Yan Li
Assistant
Computational Scientist
Computational Science
Center Brookhaven
National Laboratory

4 Alex Orlov
Associate Professor
Materials Science &
Engineering
Stony Brook University

5 Roman Samulyak
Associate Professor
Applied Math & Statistics
Stony Brook University

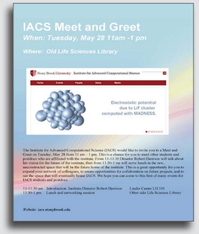
6 Steven Skiena
Professor
Computer Science
Stony Brook University

7 Allen Tannenbaum
Professor
Computer Science
Stony Brook University



Robert Panoff Shodor Education Foundation	November 15, 2013	Computational Thinking Across the Curriculum: The Power and the Peril
Martin Berzins University of Utah	October 24, 2013	Solving Multi-scale Computational Science and Engineering Problems
Tilak Agerwala and James Sexton IBM's TJ Watson Research Center	September 25, 2013	Forging Future Partnerships: IBM and SBU
J. Ilja Siepmann Stony Brook University	September 20, 2013	Computational Investigations of Phase and Sorption Equilibria
Michael Zingale Stony Brook University	September 18, 2013	Introduction to Software Engineering Practices for Scientific Computing
Philip B. Allen Stony Brook University	June 28, 2013	Computation for Crystalline Alloys – Carrier Mobility and Other Properties
Predrag Krstic University of Tennessee Knoxville	June 14, 2013	Multiscale Science for Tuning Interfaces at Nanoscale
Vincent Meunier Rensselaer Polytechnic Institute	May 23, 2013	Computational Design of Bottom-up Organic Nanoelectronics with Controlled Properties
Matthew Reuter Oak Ridge National Laboratory	April 11, 2013	Reconciling Experiment and Theory in Studies of Electron Transport

WORKSHOPS & MIXERS



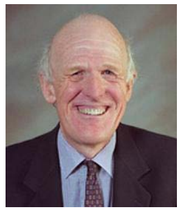
IACS Meet and Greet
May 28, 2013

August 23, 2013
GPGPU Workshop

NEWS

HANDY CLUSTER CALCULATES AT 30 TRILLION PER SECOND

New IACS high-performance computers help faculty get research results quickly



The inaugural high-performance compute (HPC) cluster of the Institute for Advanced Computational Science (IACS) at Stony Brook University is named Handy after the late Professor Nicholas Handy, Ph.D., a noted pioneer in quantum chemistry and the Ph.D. advisor of Robert Harrison, the IACS director. The new computer will be employed by Stony Brook researchers to tackle scientific challenges ranging from materials science, astrophysics, and climate science to the study of materials degrading in fusion reactors to the social sciences. The cluster, powered by processors from Intel with accelerators from both Intel and NVIDIA, is capable of performing about 30 trillion calculations per second.

The system's hardware includes 38 compute nodes (each with dual socket 2.6 GHz Xeon E5-2670 processors, 16 cores per node, and 128 GB of memory), and two high-performance file servers with a total of 320 TB of hard drive space. In addition there are two "fat" nodes configured with more memory (256 GB) to support data analysis and software development, with one "fat" node being equipped with two Intel Xeon Phi co-processors, and the other with two NVIDIA Tesla K20s.

Harrison comments, "It is very exciting to have computation finally 'happening' in the institute! While this machine will only meet a small fraction of our production computing needs, it will perhaps provide the most essential – it will be the platform on which we can rapidly and freely explore ideas and upon which our students can learn and be prepared for using the large national supercomputers."

The IACS core faculty will all be using Handy for a disparate and intriguing set of research projects. "We are using the HPC to understand the origin of liquid's water anomalies," said Associate Professor Marivi Fernandez-Serra from the Physics Department. "We need HPC to solve the very complex quantum mechanical equations that govern the motions of both electrons and nuclei. We are also using HPC to understand how water orders and behaves at the electrochemical interface. This is very important to design new electrodes for electrochemical energy storage."

Associate Professor Alan Calder, a nuclear astrophysicist from the astronomy group at SBU, will be using the cluster to help describe the nature of dense nuclear matter. We can observe the properties of neutron stars, but "interpreting the observations is difficult … because of the uncertain distances to these objects and the distortion of their spectra by high-energy processes in the atmosphere of the neutron star. The new IACS cluster, Handy, will [provide us with] the most sophisticated simulations of the atmospheres of neutron stars performed to date. These models will allow us to establish observational corrections to account for the atmosphere and thereby better constrain the fundamental theories of dense matter."

Associate Professor Arnout van de Rijt, a sociologist, will use the cluster to analyze data from mass web experiments on success-breeds-success effects (see http://iacs.stonybrook.edu/news/news-articles/does-success-breed-success). Additionally, the cluster will aid him in computationally intensive simulation models of social network dynamics. In these models large numbers of agents add and remove social ties to other agents, giving insight into the micro-level processes that may aggregate into different patterns of global connectedness.

Nicholas Handy, whose undergraduate degree was in applied mathematics, began his career as a quantum chemist in 1967 when he graduated St. Catharine's College at Cambridge University. His Ph.D. supervisor was Frank Boys who, among other things, helped established quantum chemistry as a practical computational science through the introduction of atom-centered Gaussian orbitals. Handy's own research that emphasized rigorous and practical approaches reflected his early training in applied mathematics with Boys. In 1972, Handy was appointed to the post of Demonstrator in the Theoretical Chemistry Group in the Department of Organic and Inorganic Chemistry at Cambridge. He was elected a Fellow to the Royal Society in 1990, and in 1991 he was promoted to Professor of Chemistry. After retiring from Cambridge in 2004, Handy settled in Thornthwaite in the Lake District. He died on October 2nd in 2012.

For more on Nicholas Handy, see http://en.wikipedia.org/wiki/Nicholas_C._Handy

NEWS

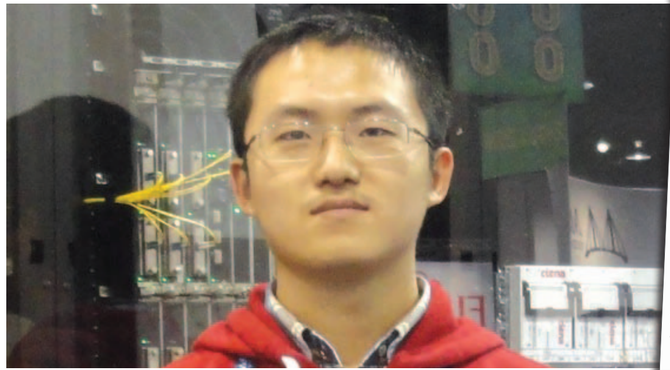
THREE SBU STUDENTS ARE CHOSEN TO PRESENT THEIR WORK AT SC13

TUESDAY, DECEMBER 17, 2013 IACS Staff | IACS funds their trip to encourage early career opportunities

Na Zhang

Three PhD Stony Brook graduate students were chosen to present their research at the SuperComputing 2013 (SC13) annual conference held this year in Denver, Colorado. Na Zhang, Chao Gao, and Yufei Ren were selected from among 36 applicants to give a talk and present a poster as part of the Doctoral Showcase Program. Here on campus, these students are from three different departments with three different advisors, but they all shared in the success of presenting their early stage work to a prestigious audience from all corners of the world.

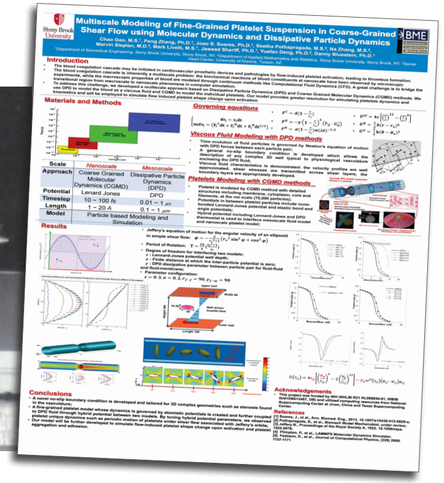
Stony Brook's Institute for Advanced Computational Science (IACS) funded their trip. "SC13 is the premiere conference worldwide in high-powered computing where all elements of the computer industry, academia and the national laboratories meet to exchange ideas and advertise their wares," said IACS Director Robert Harrison. "IACS is excited to take a leadership role in advancing computational science on a very broad front across SBU and all of SUNY, and it is a privilege to support these talented students in presenting their research and also striving to advance their careers."



Chao Gao

Each student participated in a "lightning round of short time-controlled presentations" that consisted of 4 slides with no more than 45 seconds per slide. Timing was automatic so there was no way to move to the next slide or to return to a slide. According to Alistair Rendell and Wojtek James Goscinski, the program's Chair and Co-Chair, " This is a very challenging format and it's [the student's job] to consider how to best communicate [his/her] project using images and text and tightly controlled timings."

Na is with the Applied Mathematics and Statistics Department under the tutelage of Professor Yuefan Deng. Her work involves modeling platelets. "I learned a lot [at SC13] from tutorials, workshops, great papers, posters, scientific visualizations, and the latest HPC products. Most important of all, I got a clearer idea of how the entire HPC field works: Most of the time I just work on an application, just as a user. It was a great opportunity for me to have a look at each component of supercomputers, architectures, the latest software and even to talk to technicians who work in this frontier."



Chao is with the Biomedical Engineering Department working with Professor Danny Bluestein. His work involves blood flow simulation. "My research project uses supercomputing for Biomedical research, to help understand the mechanisms of platelet activation and thrombus formation on the cellular and molecular level through multi-scale modeling and simulation. This conference helped me understand the building blocks and working mechanisms of the supercomputer so I can become a better user and fully exploit the power of supercomputers to address biomedical problems."

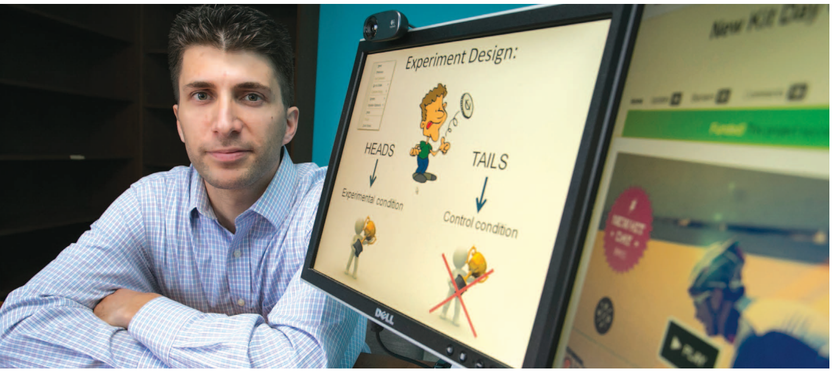
Yufei Ren

Yufei is with the Electrical and Computer Engineering Department with Dr. Dantong Yu from Brookhaven National Laboratory as his adviser. His research involves high performance data transfer and storage area networks, and he has published two technical papers, both as the first author, in SuperComputing conferences 2012 and 2013 respectively. "Attending the conference expanded my research perspective through discussing advanced research topics and exchanging fresh ideas with researchers from both academia and industry. Also I presented our group's technical paper, about high performance data transfer system, and my research to showcase our contributions to the supercomputing research community."

The Institute for Advanced Computational Science engages faculty, students and postdocs from a wide variety of academic backgrounds, all of whom have research interests that involve the use of high-performance and data-intensive computing. The pervasive entrepreneurial, think-tank culture of networking and support at IACS enables those who participate in their events to make connections that elevate careers and electrify curiosity. Students and postdocs conducting research in computational science are of particular interest to institute faculty, and every effort is made to generate support and promote opportunities to help further their careers in relevant fields. To find out more about IACS and the schedule of events, see the events tab.

DOES SUCCESS BREED SUCCESS? THURSDAY, OCTOBER 3, 2013 | SBU PRESS RELEASE

SBU Sociology Professor Arnout van de Rijt Awarded NSF Grant for Big Data Research to Get to the Bottom of An Age-Old Assumption



STONY BROOK, NY, OCTOBER 2, 2013 – Arnout van de Rijt, an associate professor in Stony Brook University's Department of Sociology and the Institute for Advanced Computational Science (IACS), has been awarded a $275,000 grant from the National Science Foundation (NSF) for his project, "Field Experiments and Formal Models of Arbitrary Social Inequality." His research focuses on success-breeds-success dynamics and suggests that many successes that individuals experience are a direct result of prior success, and not intrinsic quality or merit.

Some social scientists have proposed that one fortunate success may trigger another, the idea that success breeds success, thus producing significant degrees of arbitrary distinction between similar individuals. But evidencing this theory has been difficult because sociologists can only observe a single run of history; they cannot go back and see if the same people attain very different levels of success a second time around.

"In this NSF-funded research we overcome this problem of empirical inference through in vivo experimentation," said van de Rijt. "We sprinkle early successes at random over a population and see if the fortunate recipients end up being more successful subsequently. Because randomization ensures that the recipients are equally talented as the non-recipients, we know that any advantage the former subsequently experience relative to the latter must be due to the operation of a success-breeds-success effect. The larger this difference, the greater the extent to which successes occur arbitrarily as an accident of history."

Early results of his research were recently published in PNAS and show that when different kinds of successes (money, awards, endorsements and quality ratings) are given to arbitrarily selected recipients, all produce significant improvements in subsequent rates of success as compared to the control group of non-recipients. Link: http://www.pnas.org/content/early/2014/04/23/1316836111.full.pdf+html

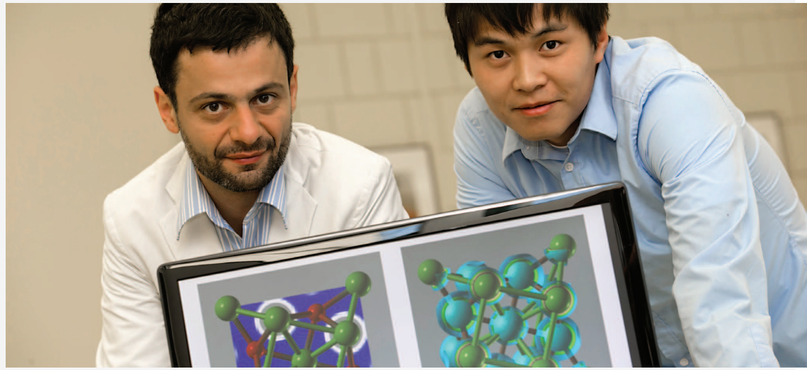
For the success-breeds-success experiments, van de Rijt is working on a computational interface that through the Internet can automatically allocate successes to large numbers of arbitrary persons and automatically record their subsequent successes. These new computing and information technologies available at Stony Brook's IACS provide unique opportunities for social scientists to conduct research that was not possible before.

"The new Institute for Advanced Computational Science does not only provide the necessary tools for such research but also brings together scholars and students from different sciences for cross-fertilization of ideas about how to use them most creatively," he added.

"My hope is that this success will breed further success," said van de Rijt. "I am lucky to have a team of very talented graduate students helping me, including junior sociologists – Michael Restivo, Idil Akin, Hyang-Gi Song – as well as computational scientists – Hua Mo. My goal is to grow this new area of sociological research, get more graduate students interested, attract more government and industry funding for it, and expand the community of scholars on campus engaged in this new, exciting field of computational social science."

SBU GEOSCIENTISTS PREDICT NEW COMPOUNDS COULD CHANGE OUR VIEW OF WHAT PLANETS ARE MADE OF

FINDINGS ESTABLISH COUNTERINTUITIVE POTENTIAL PLANET-FORMING MATERIALS | MONDAY, APRIL 22, 2013 | SBU PRESS RELEASE



A team of researchers led by Artem R. Oganov, a professor of theoretical crystallography in the Department of Geosciences, has made a startling prediction that challenges existing chemical models and current understanding of planetary interiors — magnesium oxide, a major material in the formation of planets, can exist in several different compositions. The team's findings, "Novel stable compounds in the Mg-O system under high pressure," are published in the online edition of Physical Chemistry Chemical Physics. The existence of these compounds — which are radically different from traditionally known or expected materials — could have important implications.

"For decades it was believed that MgO is the only thermodynamically stable magnesium oxide, and it was widely believed to be one of the main materials of the interiors of the Earth and other planets," said Qiang Zhu, the lead author of this paper and a postdoctoral student in the Oganov laboratory.

"We have predicted that two new compounds, MgO_2 and Mg_3O_2, become stable at pressures above one and five million atmospheres, respectively. This not only overturns standard chemical intuition but also implies that planets may be made of totally unexpected materials. We have predicted conditions (pressure, temperature, oxygen fugacity) necessary for stability of these new materials, and some planets, though probably not the Earth, may offer such conditions," added Oganov.

In addition to their general chemical interest, MgO_2 and Mg_3O_2 might be important planet-forming minerals in deep interiors of some planets. Planets with these compounds would most likely be the size of Earth or larger.

Structures of the newly predicted magnesium oxides: On the left, MgO_2; on the right, Mg_3O_2. Green – Mg atoms, red – O atoms. Isosurfaces show regions of high electron localization.

The team explained how its paper predicted the structures in detail by analyzing the electronic structure and chemical bonding for these compounds. For example, Mg_3O_2 is forbidden within "textbook chemistry," where the Mg ions can only have charges "+2," O ions are "-2, and the only allowed compound is MgO. In the "oxygen-deficient" semiconductor Mg_3O_2, there are strong electronic concentrations in the "empty space" of the structure that play the role of negatively charged ions and stabilize this material. Curiously, magnesium becomes a d-element (i.e. a transition metal) under pressure, and this almost alchemical transformation is responsible for the existence of the "forbidden" compound Mg_3O_2.

The findings were made using unique methods of structure prediction, developed in the Oganov laboratory. "These methods have led to the discovery of many new phenomena and are used by a number of companies for systematically discovering novel materials on the computer — a much cheaper route, compared to traditional experimental methods," said Zhu.

"It is known that MgO makes up about 10 percent of the volume of our planet, and on other planets this fraction can be larger. The road is now open for a systematic discovery of new unexpected planet-forming materials," concluded Oganov.

This work is funded by the National Science Foundation and DARPA.

IACS IS ON THE MOVE

We are less than a year away from moving into our newly renovated space in the Old Life Sciences Library, that also houses the Laufer Center. Features of this new space include a 45-seat multi-purpose room, 18 offices; a full-service kitchen, two conference rooms and a 35-seat open area for graduate students. In the multi-purpose space, the conference rooms and the Director's office there will be state-of-the-art AV systems including multifunctional overhead and LCD screens

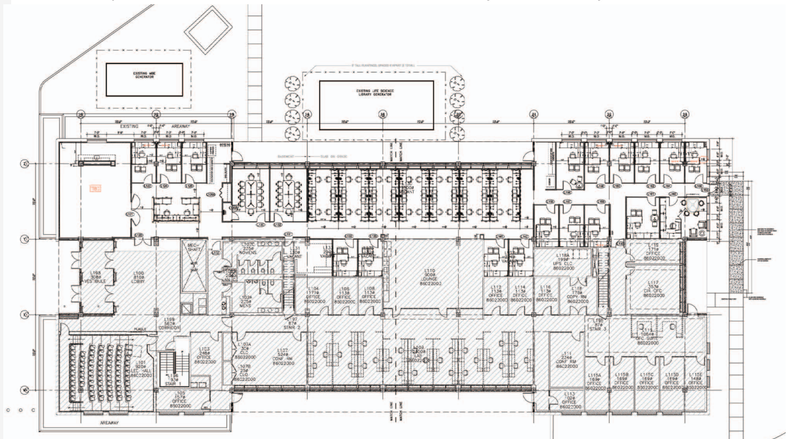
THE INTENT OF THE SPACE IS TO CULTIVATE THE EXCHANGE OF IDEAS ACROSS DISCIPLINES AND TO ENCOURAGE FORWARD-THINKING.

with both professional and desktop video conferencing capabilities supported. The intent of the space is to cultivate the exchange of ideas across disciplines and to encourage forward thinking in a highly collaborative environment where members and visitors will have access to a wide range of resources. Construction is slated to begin in mid 2014 with a move-in date proposed for spring 2015.

Open Administration Area

Graduate Student Seating

Large Private Office



Mid-size Private Office

Small Private Office

Director's Office

FUTURE PLANS

The coming year holds much promise and excitement. As a result of our recruiting efforts, which discovered some truly outstanding senior and junior candidates, we are looking forward to beginning the fall of 2014 with at least two new faculty members and the possibility of several more. Our new colleagues will bring new vantage points and energies to IACS and

MULTIPLE PARTNERSHIPS WITH LEADING TECHNOLOGY COMPANIES AND NEW YORK STATE INDUSTRIES ARE EXPECTED TO BEAR FRUIT IN THE COMING YEAR

will play critical roles in further establishing IACS as a vibrant multidisciplinary institute. Coming on board in the same time frame is our new professional system administrator and our HPC2 (http://hpc2.org) program manager. Together, these hires bring our headcount up to at least 10 core faculty, 14 affiliate faculty, two research faculty, one administrative director plus a part-time assistant, two technical staff, and 29 students and postdocs, with professional staff under subcontract for graphics design, web development and proposal writing.

In late fall 2014 we will be deploying a large expansion of our high-performance computer capability as a result of the grant from LIRED. A cluster that is at least 4x more powerful than our current system will be installed at BNL. This will be connected via fast networking to IACS's own system that in turn will be expanded with several powerful servers equipped with very large memory for data analysis and to support rapid prototyping and experimental computing. These resources are essential to many of our ambitions, including engagement with local industries under the HPC2 program. Multiple partnerships with leading technology companies and New York State industries are expected to bear fruit in the coming year, catalyzed by collaborations that span the state and include BNL.

Our graduate program committee, that has been leading the charge to develop a campus-wide approach to graduate-level education and training in computational science, will be taking concrete steps to establish a graduate certificate including new program tracks and courses. Challenging us to think big is the vision of expanding this to include data-science, bringing the power of "big data" into the hands of our young scientists. Complementing this will be an expansion of the highly popular workshops at SBU in HPC programming offered by IACS together with staff from BNL's Computational Science Center.

And last, but by no means least, we will be moving into our new space very early in 2015, and we will mark this milestone with multiple events and celebrations.

FELLOWSHIPS OFFERED

IACS now offering fellowships to new recruits and junior researchers

NEW RECRUITS: In an effort to attract the best and brightest to SBU and to work with faculty within IACS, we have created the IACS New Recruit Fellowship which allows for a stipend of $32,000 plus $4000 for travel and equipment. Students are selected by their home departments based on their outstanding potential indicated, for instance, by high undergraduate GPA, strong letters of recommendation, as well as their active research record.

JUNIOR RESEARCHERS: This fellowship is awarded to continuing graduate students who are conducting full-time research and are recognized as outstanding junior researchers by institute faculty or affiliates. Those who apply must write a 2-page research statement and give a 30-minute presentation to the IACS community and the fellowship committee. The fellowship allows for a stipend of $32K for up to three calendar years, plus $4K per year for travel and equipment. The faculty members or affiliates supervising the students receive an additional $3K in relief funds.

GPGPU

Institute holds its first tutorial workshop

The Institute for Advanced Computational Science held its first computing workshop on Friday, August 23, 2013 from 9-5 pm. Participants learned about GPGPU programming in an all-day session that included training led by staff from the Center for Computational Science at Brookhaven National Laboratory. The morning session centered on Programming with GPGPUs followed by lunch and four case studies: GPU Implementation of Lagrangian Particle Methods for Compressible Euler Equations; GPU Acceleration for Medical Imaging and Visualization; Survey of Techniques on Medical Imaging Computation; and GPUs versus CPUs . Attendance and lunch were free and over 75 students and staff participated.

ANNUAL DINNER HELD

50 guests attend 1-year anniversary celebration

As a way of commemorating our first full year as an institute, the IACS held a celebratory dinner at The Fifth Season restaurant in Port Jefferson on December 3. The event was a rousing success with over 50 people attending. In recognition of the vision and significant contribution of university leadership and faculty to our success as a fledgling institute, we invited those people from both SBU and Brookhaven National Laboratory who played, and are still playing, an active role in supporting our efforts to establish roots while growing our faculty and resources. Some of the notable guests who attended were Provost Dennis Assanis, Associate VP for Brookhaven National Laboratory Affairs Peter Paul, Chief Information Officer Cole Camplese, Senior Vice President for Administration Barbara Chernow, and former Vice President for Research Benjamin Hsiao.

IACS IS HIRING

Five tenure-track faculty and two staff positions available

Five tenure-track faculty positions are open and presently being advertised within the institute – three at the assistant professor level and two at the full professor level, the latter with named chairs and significant individual endowments. In addition to hiring new faculty, IACS is looking for two new staff members. The institute has an opening for a Research IT Engineer to oversee and manage the new Handy computer cluster recently purchased, as well as an opening for a Senior Research Support Specialist to lead the High Performance Computing Consortium (HPC2), a project funded by New York state in collaboration with Rensselaer Polytechnic Institute, SUNY Buffalo, and Icahn School of Medicine at Mount Sinai.

AWARDS CREATED

IACS creates two new awards for students

YOUNG WRITER'S AWARD: The IACS Young Writer's Award is granted to a graduate or undergraduate student working with a faculty member or affiliate of the institute. The award consists of a one-time prize of $500 to celebrate the student's first paper that is accepted in a peer-reviewed publication.

TRAVEL AWARD: The IACS Travel Award is granted to graduate students and postdocs who are working with faculty or affiliates of the institute. This award reimburses travel costs associated with international scientific or professional conferences or meetings, up to a maximum of $2,000. Granting of the award requires that the student present his or her research at the event.

CURRENT EVENTS

December 20, 2013 (Artem Oganov)
SBU Team Discovers New Compounds that Challenge the Foundation of Chemistry
Breakthrough may lead to novel materials and applications

December 17, 2013
Three SBU students are chosen to present their work at SC13
IACS funds their trip to encourage early career opportunities

December 13, 2013
Big, Bigger, Biggest?
Steven Skiena's Algorithms Help Answer the Questions

October 3, 2013
Does Success Breed Success?
SBU Sociology Professor Arnout van de Rijt Awarded NSF Grant for Big Data Research to Get to the Bottom of An Age-Old Assumption

April 22, 2013 (Artem Oganov)
SBU Geoscientists Predict New Compounds Could Change Our View of What Planets are Made of
Findings establish counterintuitive potential planet-forming materials

April 15, 2013 (Artem Oganov & Alexander Orlov)
SBU Professors Collaborate on NSF-Funded 'Materials Genome Initiative'
White House supported initiative to speed up transition time from lab to marketplace

March 29, 2013 (Arnout van de Rijt)
SBU Led Research Finds That Most Fame Isn't Fleeting

FUNDING

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DARPA
U.S. ARMY RDECOM TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.
Colorado State University
U.S. DEPARTMENT OF ENERGY
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EMPIRE INNOVATION PROGRAM

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1 Alan C. Calder Associate Professor

Alan Calder is an associate professor in the Department of Physics and Astronomy at SBU. His research is in the field of nuclear astrophysics, and his work involves simulating explosive astrophysical phenomena. Prior to coming to Stony Brook, he had research appointments at the National Center for Supercomputing Applications and the University of Chicago. His research is principally in bright stellar explosions known as Type Ia supernovae. The light curves of these events can be standardized and thereby used as distance indicators for cosmology studies investigating the expansion history of the Universe.

2 Rezaul Alam Chowdhury Assistant Professor

Rezaul Chowdhury is an assistant professor in Computer Science at Stony Brook University. Prior to joining SBU he worked with the Structural Bioinformatics Group at Boston University, and the SuperTech Research Group at MIT. Before moving to Boston he was a postdoctoral fellow at the Center for Computational Visualization, Institute for Computational Engineering & Sciences at the University of Texas at Austin. He received his PhD in Computer Sciences also from UT Austin working with the Theory group.

3 Marivi Fernandez-Serra Associate Professor

Marivi Fernandez-Serra is an associate professor in the Department of Physics and Astronomy at SBU. She received her PhD in 2005 from the University of Cambridge and then worked as a postdoc at the Center for Atomic and Molecular Simulations in Lyon, France. Her research is in the field of computational condensed matter physics. She develops and applies methods to study the atomic and electronic dynamics of complex materials. One of her main research areas is the study of fundamental properties of liquid water using quantum mechanical simulations. In 2010 she was awarded a DOE Early Career award to develop methods to simulate liquids under non-equilibrium conditions.

4 Robert J. Harrison Professor and Director

Robert Harrison is a professor of Applied Math and the director of the Institute for Advanced Computational Science at SBU. He is also the head of the Computational Science Center at BNL. Dr. Harrison comes to Stony Brook from the University of Tennessee and Oak Ridge National Laboratory, where he was the Director of the Joint Institute of Computational Science, Professor of Chemistry and Corporate Fellow. He has a prolific career in high-performance computing with over one hundred publications on the subject, as well as extensive service on national advisory committees,


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5 Xiangmin Jiao Associate Professor

Dr. Jiao received his B.S. in 1995 from Peking University, China, his M.S. in 1997 from University of California Santa Barbara, and his Ph.D. in computer science in 2001 from University of Illinois at Urbana-Champaign (UIUC). After working in interdisciplinary research for a few years as a Research Scientist at the Center for Simulation of Advanced Rockets (CSAR) at UIUC and then as a Visiting Assistant Professor in College of Computing at Georgia Institute of Technology, he joined the faculty of Stony Brook University in Fall 2007. He is now an Associate Professor in the Department of Applied Mathematics and Statistics and is affiliated with the Computer Science Department.

6 Marat Khairoutdinov Associate Professor

Associate Professor Marat Khairoutdinov obtained his Ph.D. degree in 1997 from the University of Oklahoma. From there he was employed as a Research Scientist at Colorado State University and then came to Stony Brook's School of Marine and Atmospheric Sciences in 2007. During his Ph.D. studies, he developed one of the first Large-Eddy Simulation (LES) models with explicit/bin microphysics and applied it to study the evolution of drizzling marine stratocumulus clouds. After graduating, he redesigned his LES model to handle deep convective clouds and made it suitable to run on massively parallel computers. The new cloud-resolving model named System for Atmospheric Modeling, or SAM, has been applied to various interesting convection problems and is being used by scientists in their research at a wide variety of institutions.

7 Artem R. Oganov Professor

Professor Artem Oganov received his PhD in Crystallography from the University College London in 2002. He was a Group Leader at ETH Zurich from 2003-2008, at which time he came to Stony Brook as an Associate Professor and then became a full professor in 2010. His career record boasts over 122 papers published, one book, 2 patents, and he has given over 200 talks and colloquia. Professor Oganov is on the Editorial Board member of the "Journal of Superhard Materials" and "Scientific Reports" (Nature Publishing Group), he has refereed for more than 60 journals and for Oxford University Press book publishing, and he is the founder and chairman of the Commission on Crystallography of Materials (International Union of Crystallography). Most recently he has become the Director of the Center for Materials by Design at Stony Brook University.

8 Arnout van de Rijt Associate Professor

Associate Professor Arnout van de Rijt received his PhD from Cornell University. He came to the Sociology Department at Stony Brook University in 2007, and in 2013 he was granted tenure. His research interests include Social Networks, Collective Action, Cumulative Advantage, Mathematical Sociology, and Computational Methods. For his contributions to social network analysis he received the 2010 Freeman Award for Distinguished Junior Scholarship and several best article awards. His research is supported by the National Science Foundation and has been published in American Sociological Review and American Journal of Sociology.

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VISITORS 2013

December	Yukina Yokoi	Graduate Student	Toyohashi University of Technology
November	Robert Panoff	Executive Director	Shodor Education Foundation
October	Martin Berzins	Professor	University of Utah, SCI institute
September	Zachary Giles	HPC Systems Administrator	Mount Sinai School of Medicine
September	Tilak Agerwala	VP Data Centric Systems	IBM TJ Watson Research Center
September	James Sexton	Program Director CSC	IBM TJ Watson Research Center
June	Predrag Krstic	Professor	University of Tennessee Knoxville
May	Vincent Meunier	Associate Professor	Rensselaer Polytechnic Institute
April	Matthew Reuter	Wigner Fellow	Oak Ridge National Laboratory
April	Bryan Sundahl	Graduate Student	University of Tennessee Knoxville
April	Deborah Penchoff	Graduate Student	University of Tennessee Knoxville
April	Scott Thornton	Research Scientist	JICS, Oak Ridge National Laboratory

STUDENTS

1 Afife Idil Akin
PhD Student

2 Rebecca Conley
PhD Student

3 Tristan Delaney
PhD Student

4 Daniel Elton
PhD Student

5 Lonia Friedlander
PhD Student

6 Pramod Ganapathi
PhD Student

7 Prankur Gupta
MS Student

8 Sarang Joshi
MS Student

9 Jungmin Lee
PhD Student

10 Hongxu Liu
PhD Student

11 Yue Liu
MS Student

12 Cao Lu
PhD Student

13 Sumit Malik
MS Student

14 Hua Mo
PhD Student

15 Pavan Narasimhaprasad
MS Student

16 Betül Pamuk
PhD Student

17 Guangrui Qian
PhD Student

18 Navamita Ray
PhD Student

19 Michael Restivo
PhD Student

20 Hyang-Gi Song
PhD Student

21 Adrian Soto
PhD Student

22 Bryan Sundahl
PhD Student

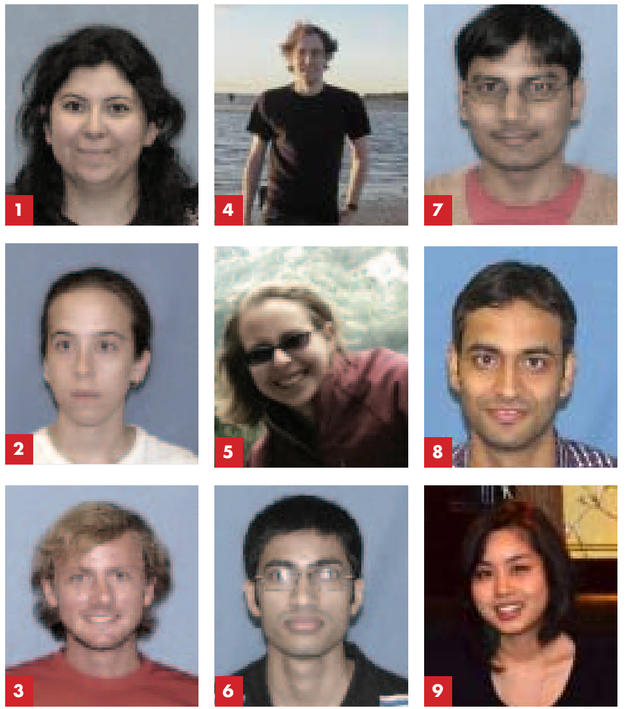
23 Jesmin Jahan Tithi
PhD Student

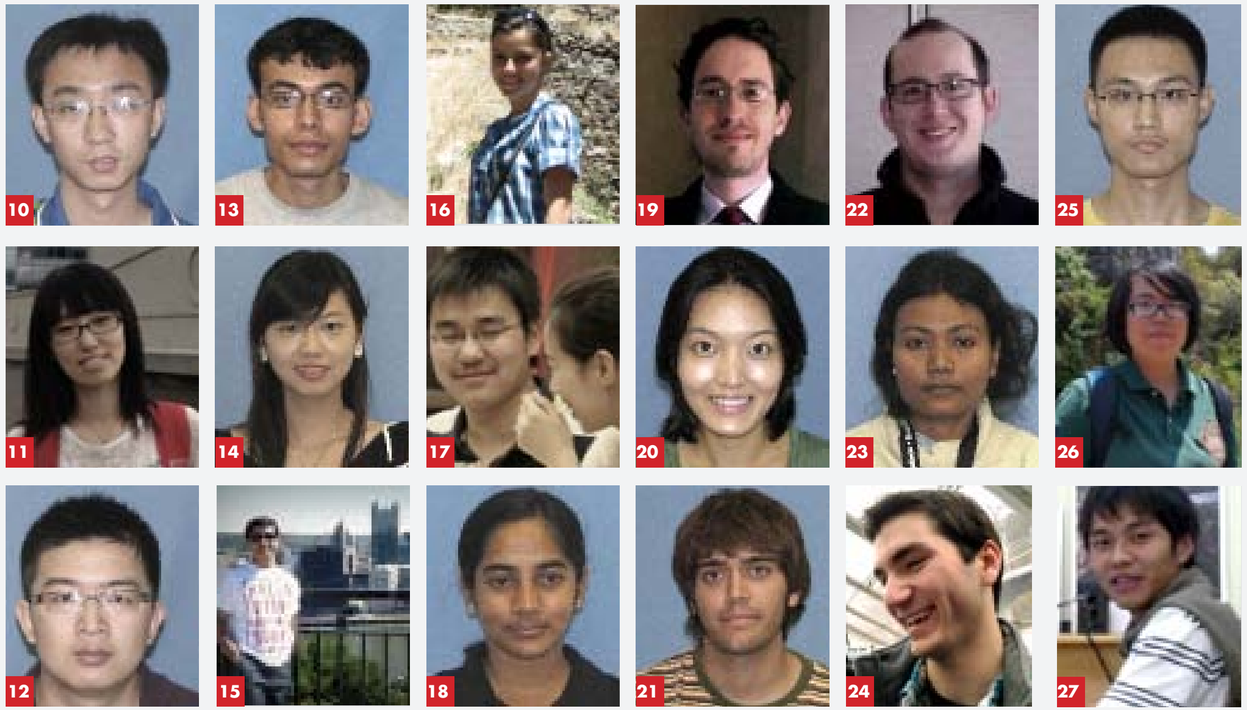
24 Joe Trollo
Undergraduate

25 Xiongfei Wei
MS Student

26 Hongfei Xu
MS Student

27 Qiang Zhu
PhD Student





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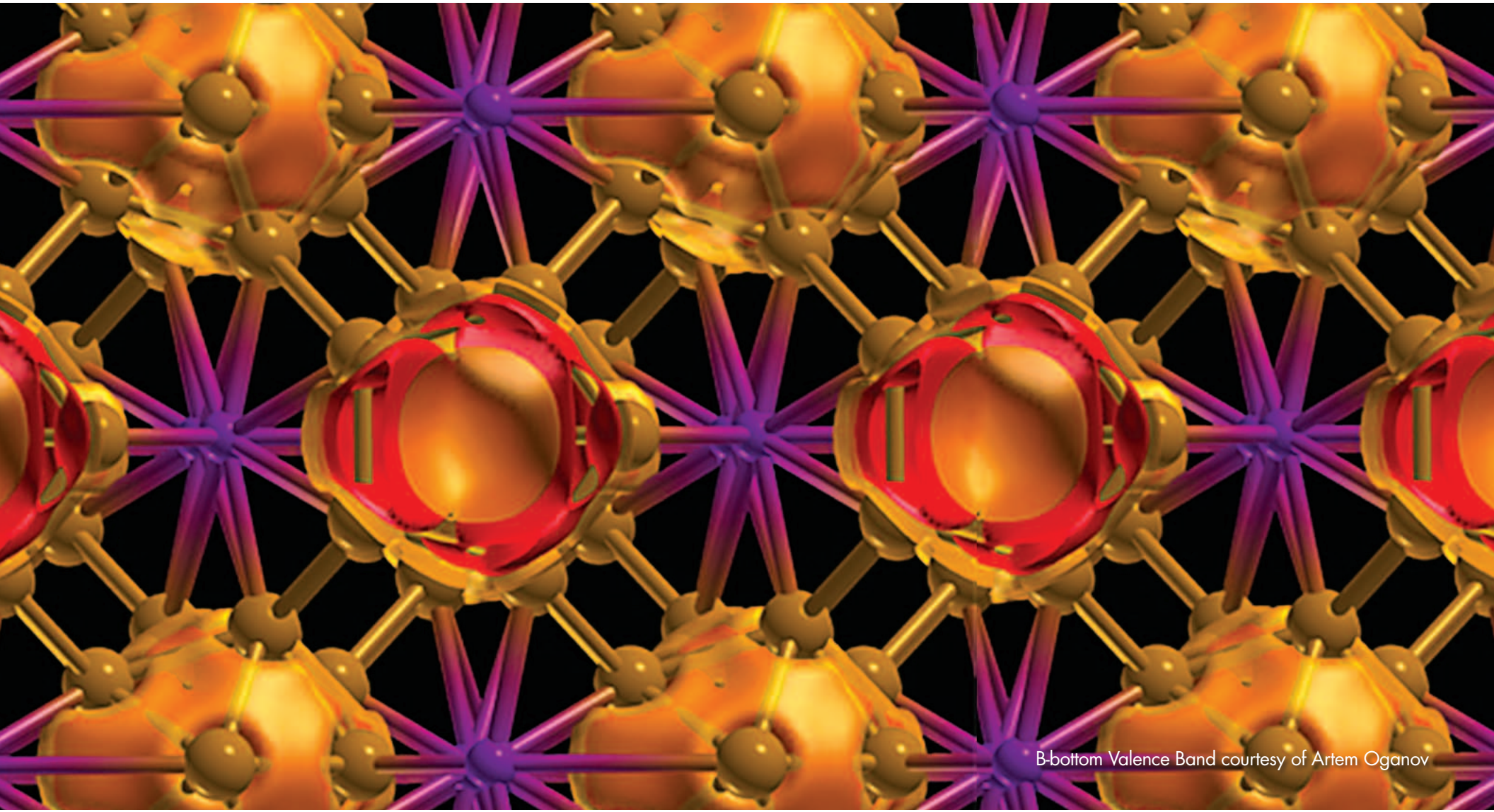

B-bottom Valence Band courtesy of Artem Oganov

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