
ISDSB 2016, Knoxville, TN, August 07, 2016
Jack Johnson


Robert Phillips
Andrey Kovalevsky


Lays




NSLS-II biomedical beamlines for micro-crystallography, FMX,
and for highly automated crystallography, AMX:
New opportunities for advanced data collections.
ISDSB 2016, Knoxville, TN, August 07, 20
Yota Fukuda
Taro Tamada


Steven Dajnowicz
Christopher Goins
Bryant Hanson






Welcome to the
5th International Symposium on
Diffraction Structural Biology
ISDSB2016
Knoxville, Tennessee, USA
OAK RIDGE National Laboratory
HIGH FLUX ISOTOPE REACTOR
SPALLATION NEUTRON SOURCE
Hilton
Knoxville


Molecular Dimensions
UVEX UV
MICROSCOPES FOR PROTEIN CRYSTAL DETECTION
• Manual to fully automated versions with storage
• Sensitive camera and optics for excellent image quality
• Very high resolution for detection of microcrystals 1 micron or smaller
• UV fluorescence for identifying protein crystals and transmission for nucleic acid crystals
Molecular Dimensions


Art Robbins Instruments
Crystal Gryphon
A personal sized version of the Phoenix.
The small, fast, affordable way to set up all your plates.
Set up sitting drop, hanging drop and microbatch plates.
The Crystal Phoenix is now available with 1, 2, 3 or 4 protein dispenser channels to fill more wells in less time.
Gryphon Liquid Handling System
Features:
Scorpion
ARI
John Clemente


Rigaku
oxford diffraction
CRYSTALLOGRAPHY
LECULAR CRYSTALLOGRAPHY
L SAXS
Charlie Pemble


OAK RIDGE National Laboratory
High Flux Isotope Reactor
The highest-flux reactor-based source of neutrons in the US for research to study materials
Researchers are developing novel neutron spin-echo techniques for high-resolution spectroscopy at HFIR.
Neutron radiography and computed tomography allowed researchers to nondestructively study the internal structures of gasoline fuel injectors.
Neutrons were used to describe how a high-temperature superconducting material
OAK RIDGE National Laboratory
Second Target Station
A high-brightness pulsed source optimized for cold neutrons
Researchers will be able to exploit the magnetic interaction of neutrons with matter to unravel the structure and dynamics arising in complex magnetic materials.
Researchers will be able to simultaneously probe the structure and function of complex materials across broader length and time scales.
Experiments with smaller samples will become possible using high-brightness cold neutrons.
OAK RIDGE National Laboratory
Spallation Neutron Source
The most intense pulsed accelerator-based neutron beams in the world to study materials
Neutrons helped to reveal details about a classic transition-metal oxide, vanadium dioxide, by quantifying the thermodynamic forces driving the transformation.
Neutron scattering measurements confirmed plutonium's magnetism, which scientists have long theorized but have never been able to experimentally observe.
OAK RIDGE National Laboratory
HIGH FLUX ISOTOPE REACTOR
SPALLATION NEUTRON SOURCE




Hilton
Knoxville


Hilton
Knoxville
Wah Chiu


Protein Backbone Traced in CryoEM Maps
Hilton Knoxville
EXIT


Ichiro Tanaka


Hilton
Knoxville


IMAGINE beam line at HIFR
HFIR cold guide hall
CG4 beam line end position
Neutron spectrum transmitted by CG-4: 2 Å – 10 Å
EXIT
Hilton Knoxville


6th International Symposium on
Diffraction Structural Biology
August 7-10, 2016
Troy Wymore


Extracellular Polysaccharides Perform Vital Functions in Life
Hyaluronan
Cellulose
Alginate
Chitin
Hilton
Knoxville
EXIT

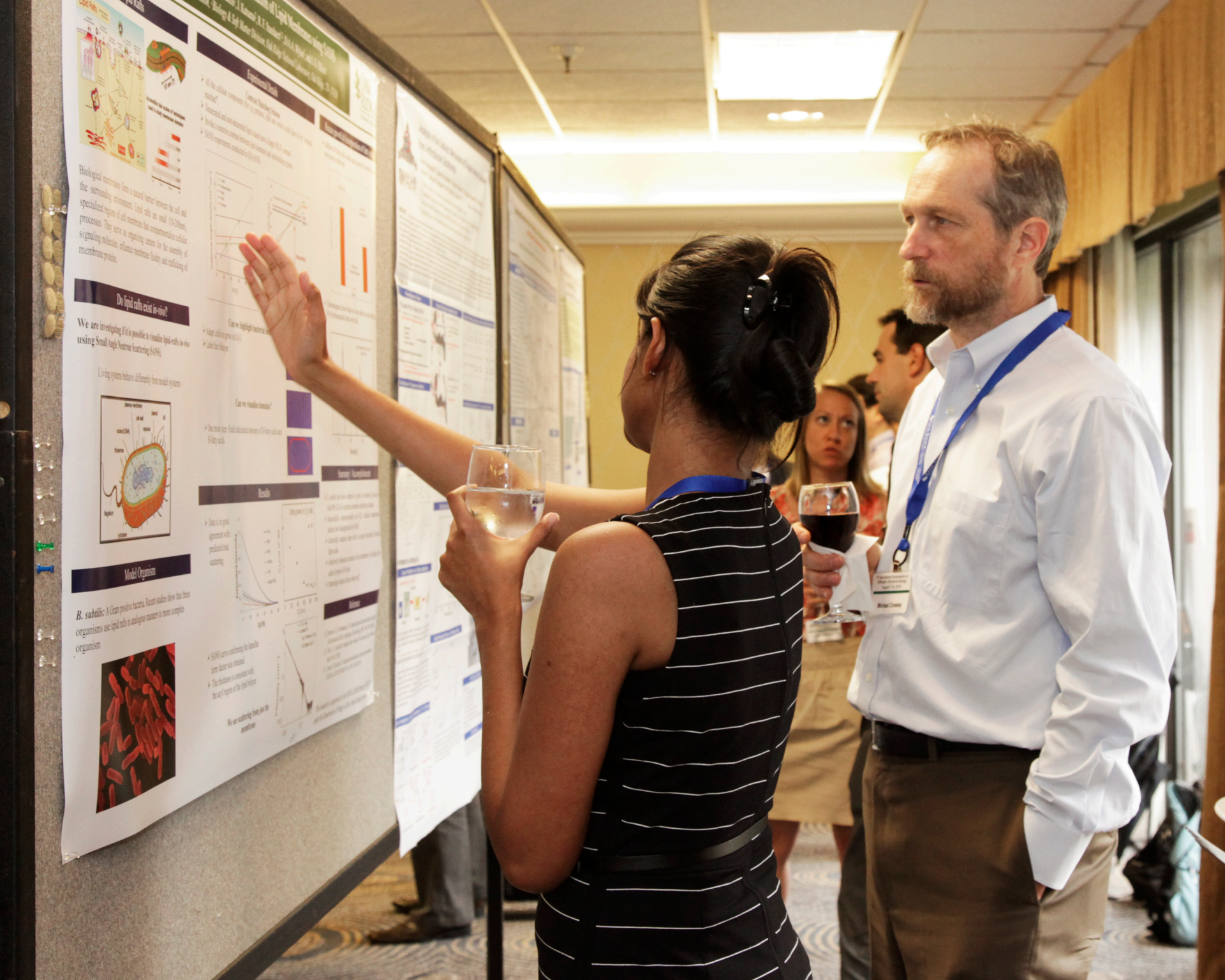










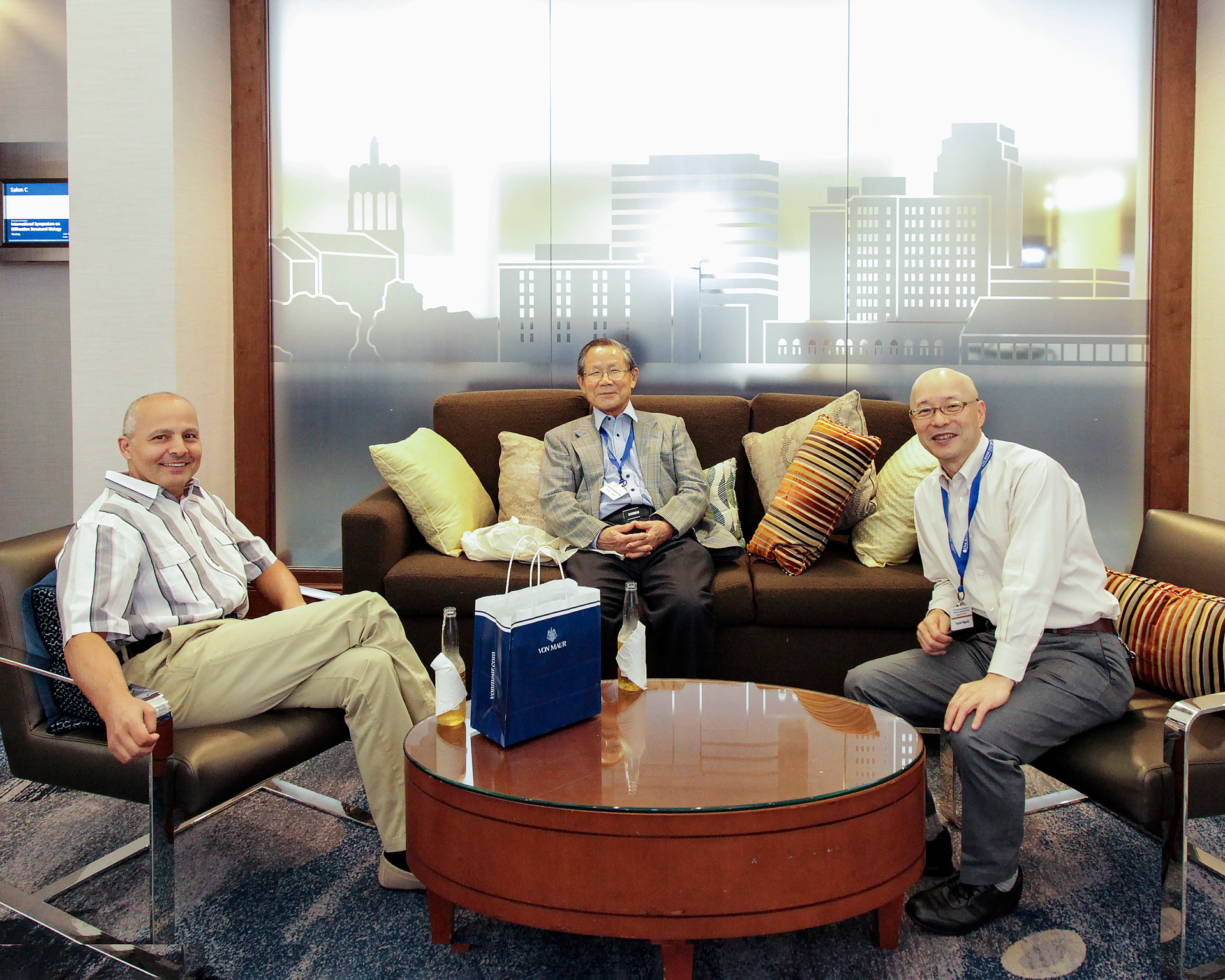

Lipid Rafts
Biological membranes form a natural barrier between the cell and the surrounding environment. Lipid rafts are small (10-200nm), specialized regions of cell membrane that compartmentalize cellular processes. They serve as organizing centers for the assembly of signaling molecules, influence membrane fluidity and trafficking of membrane proteins.
Do lipid rafts exist in-vivo?
We are investigating if it is possible to visualize lipid-rafts in-vivo using Small Angle Neutron Scattering (SANS).
Living systems behave differently from model systems
Model Organism
B. subtilis: A Gram positive bacteria. Recent studies show that these organisms use lipid rafts in analogous manners to more complex organism
Experiment Results
Results
Summary / Accomplishment
Reference


Rigaku
oxford diffraction
CHEMICAL CRYSTALLOGRAPHY
MACROMOLECULAR CRYSTALLOGRAPHY
BIOLOGICAL SAXS
OAK RIDGE
National Laboratory
Isotope Reactor
OAK RIDGE
National Laboratory
Second Target Station
A high-brightness pulsed source optimized for cold neutrons
OAK RIDGE
National Laboratory
HIGH FLUX ISOTOPE REACTOR
SPALLATION NEUTRON SOURCE


An effective deuterium exchange method for a neutron structure analysis by use of unfolding-refolding processes.
Akiko Kita and Yukio Morimoto (Research Reactor Institute, Kyoto University)
Investigating the Multiple Functions of Dehaloperoxidase Through Ligand Binding and H-bonding Networks: An X-ray and Neutron Crystallographic Study
ABSTRACT
Established substrate binding sites
2,4-dihalophenol (DCP & DBP) binding and reactivity
Peroxidase substrates
2,4,6-trihalophenol (Cl, Br)
Preliminary neutron diffraction results
Conclusions


5th International Symposium on
Diffraction Structural Biology
August 7-10, 2016




Salon C
VON MAUR
vonmaur.com


EXIT
EXIT




NEUTRONS 2025
OAK RIDGE
Gregory Hura




Rigaku
OAK RIDGE
National Laboratory
High Flux Isotope Reactor
Oksana Gerlits


NEUTRONS BLOSS
OAK RIDGE






EXIT
EXIT






ography, AMX:
ata collections.
Knoxville, TN, August 07, 2016
Hilton
Knoxville


EXIT






Themes: Great things coming together
NATIONAL RENEWABLE ENERGY LABORATORY
Hilton
Knoxville
EXIT


XIAOHU HU
Characteristic Time versus Observation Time
Experiments
MD data
$\log_{10}(\tau_c/10^{-12}$ s)
$\log_{10}(t/10^{-12}$ s)
0 2 4 6 8 10 12 14 16
12 10 8 6 4 2 0 −2
PGK domains
PGK residues
K-RAS segments
ePepN, dom. 1-2
ePepN, dom. 2-3
ePepN, dom. 2-4
ePepN, dom. 4-rest
Ref. 3
Ref. 4
$\propto t^{0.9}$
Nature Physics 12 171 (2016)


Hilton




Hilton
Knoxville