CUI THE HAMBURG CENTRE FOR ULTRAFAST IMAGING

The Hamburg Centre for Ultrafast Imaging

International Symposium 2014

Hamburg

Campus Bahrenfeld, CFEL

November 12 – 14

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

DESY

EMBL

MAX-PLANCK-GESELLSCHAFT

European XFEL

Program

Wednesday, November 12, 2014

10:00 Registration/Coffee

10:30 **Ole Krogh Andersen**
Band structures of cuprate superconductors and nickelate magnets

11:30 **Anna Krylov**
Electronic resonances: an equation-of-motion coupled cluster based approach

12:30 Lunch Break

14:00 **Matthias Weidemüller**
Simulating dipolar energy transport with giant atoms

15:00 **Dmitri Golberg**
Nanomaterial properties as revealed by in-situ *transmission electron microscopy*

16:00 Coffee Break

16:30 Poster Session

17:00 Welcome Reception (Poster Session cont.)

Thursday, November 13, 2014

9:00 **Thomas Irving**
Time-resolved diffraction and scattering from non-crystalline biological materials: present status and future prospects

10:00 Coffee Break

10:30 **Thomas Marlovits**
Visualizing molecular machines

11:30 **Cristiane Morais Smith**
Engineering quantum states of matter in cond-mat and cold-atom systems

12:30 Lunch Break

14:00 **Tilman Esslinger**
Bands with a twist and quantum sized steps

15:30 Prize Session
"***Hamburger Preis für theoretische Physik***"
Laudation: **Thierry Giamarchi**
Laureat's Talk
Antoine Georges

Friday, November 14, 2014

9:00 **Martin Caffrey**
In meso in situ serial femtosecond crystallography of membrane (and soluble) proteins

10:00 Coffee Break

10:30 **Thierry Giamarchi**
Local quenches and mobile impurities in cold atomic gases

11:30 **Patanjali Kambhampati**
Excitons in semiconductor quantum dots: Design principles for lasers, optical switches, and LEDs

12:30 Lunch Break

14:00 Joint Session of PIER Photon Science Colloquium and CUI Symposium

14:00 **Hubert Ebert**
Angular momentum resolved photoemission in one step: Recent developments in theory

15:15 **Majed Chergui**
Tracking the electron in molecular systems and solid materials

Program Award Ceremony, November 13

15:30 Welcome Address
Petra Herz
Chairwomen of the Executive Board, Joachim Herz Foundation

Welcome Address
Dr. Dorothee Stapelfeldt
Second Mayor and Senator for Science and research of Hamburg

Interview
Ralf Krauter
Science journalist
Prof. Klaus Sengstock
Spokesperson of The Hamburg Centre for Ultrafast imaging (CUI)
Prof. Albrecht Wagner
Member of the Board of Trustees of Joachim Herz Foundation

Laudatio
Prof. Thierry Giamarchi
Université de Genève

Interview
Ralf Krauter, *science journalist*, and
Prof. Antoine Georges

Presentation of the Award to
Prof. Antoine Georges

16:30 Reception

17:00 Lecture
Prof. Antoine Georges

Location, contact and directions

Location

Campus Bahrenfeld
Notkestraße 85 (Main Entrance)/Luruper Chaussee 149 (Side Entrance)
Building 99 (CFEL), Foyer Seminar-room I - III

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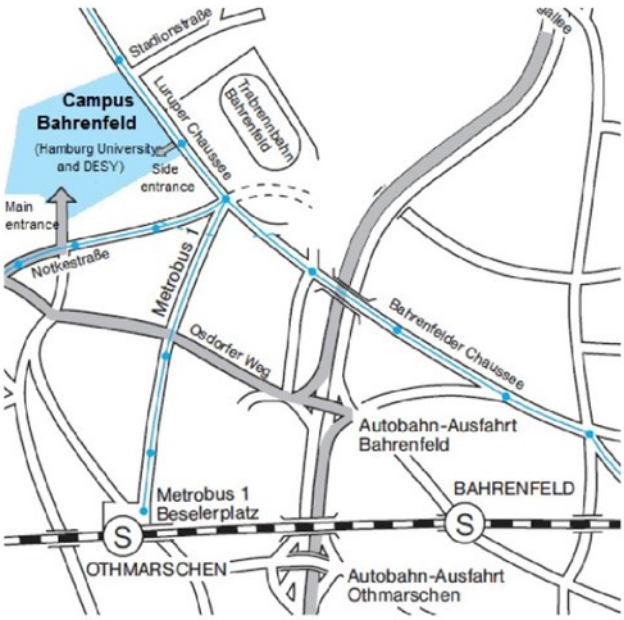
Directions:



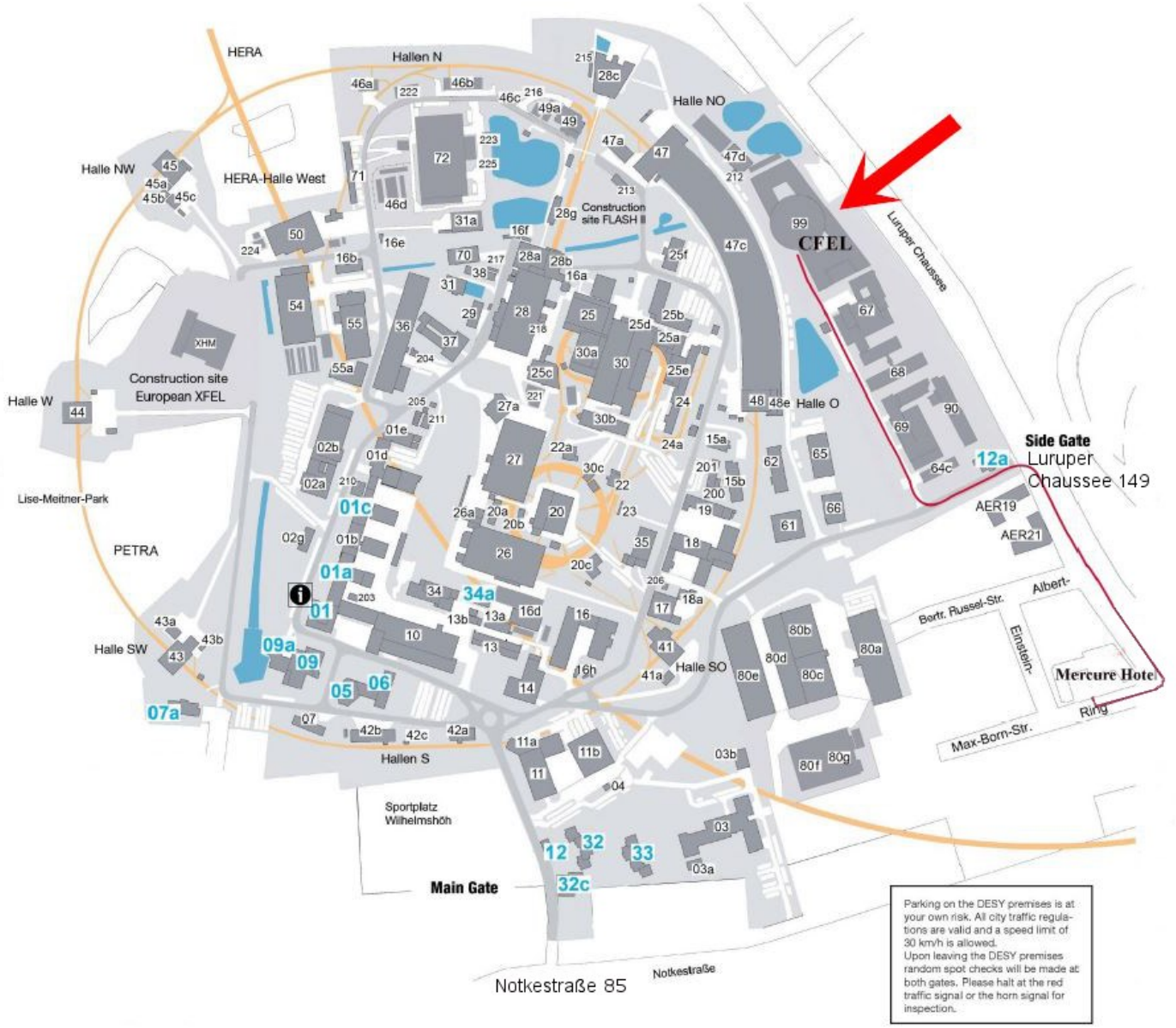
By train: to Hamburg-Altona station, then continue by taxi (travelling time ~15min) or take a bus (see below).

By bus: To reach the side gate (recommended), take bus line 2 (direction Schenefeld Mitte) from Altona train station and get off at "Luruper Chaussee/DESY", travelling time ~20min.

From train station "S-Bahn Othmarschen", take bus line 1 (direction "Schenefelder Holt") directly to the main entrance of the campus (bus stop "Zum Hünengrab/DESY"), traveling time ~25 min.

By plane: The campus can be reached from Hamburg airport by taxi in ~30min. Alternatively, take suburban train S1 to Altona or Othmarschen (~40min, direct train) and a bus from there (see above).

Campus Map


HERA
Hallen N
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HERA-Halle West
Construction site FLASH
CFEL
Luruper Chaussee
Halle W
Construction site European XFEL
Halle O
Side Gate
Luruper Chaussee 149
Lise-Meitner-Park
PETRA
AER19
AER21
Halle SW
Halle SO
Bertr.-Russel-Str.
Albert-Einstein-Ring
Mercure Hotel
Max-Born-Str.
Hallen S
Sportplatz Wilhelmshöh
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List of invited Speakers

Ole Krogh Andersen (Max-Planck-Institut für Festkörperforschung, Stuttgart)
Explaining the basic band structures of cuprate superconductors and nickelate magnets

Martin Caffrey (Trinity College Dublin, Dublin)
In meso in situ serial femtosecond crystallography of membrane (and soluble) proteins

Majed Chergui (École polytechnique fédérale de Lausanne, Lausanne)
Tracking the electron in molecular systems and solid materials

Hubert Ebert (Ludwig-Maximilians-Universität, München)
Angular momentum resolved photoemission in one step: Recent developments in theory

Tilman Esslinger (Eidgenössische Technische Hochschule Zürich, Zürich)
Bands with a twist and quantum sized steps

Antoine Georges (Collège de France & École Polytechnique, Paris; Université de Genève, Genève)
Prize lecture

Dmitri Golberg (Center for Materials Nanoarchitectonics (MANA), Natianal Institute for Materials Science (NIMS), Tsukuba, Japan)
Nanomaterial Properties as Revealed by in-situ Transmission Electron Microscopy

Thierry Giamarchi (Université de Genève, Genève)
Local quenches and mobile impurities in cold atomic gases

Thomas Irving (Illinois Institute of Technology, Chigago))
Time-Resolved Diffraction and Scattering from Non-Crystalline Biological Materials: Present Status and Future Prospects

Patanjali Kambhampati (McGill University, Montreal, Canada)
Excitons in Seminconductor Quantum Dots: Desighn principles for lasers, optical switches, and LEDs

Anna Krylov (Universtiy of Southern California, Los Angeles, USA)
Electronic Resonances: An Equation-of-Motion Coupled-Cluster Based Approach

Thomas Marlovits (Institut für Molekulare Biotechnologie, Wien)
Visualizing molecular machines

Cristiane Morais Smith (Universiteit Utrecht, Utrecht)
Engineering quantum states of matter in cond-mat and cold-atom sytems

Matthias Weidemüller (Ruprecht-Karls-Universität, Heidelberg)
Simulating dipolar energy transport with giant atoms

Speakers' abstracts

Ole Krogh Andersen (Max-Planck_Institut für Festkörperforschung, Stuttgart)

Band structures of cuprate superconductors and nickelate magnets

The cuprates which superconduct upon hole doping all have electronic configuration $3d^9$ and layered, perovskite-derived crystal structures. They all have the same temperature-vs-doping phase diagram which, at low temperature, starts with an antiferromagnetic, insulating phase, followed by a bad-metallic phase, then the superconducting phase, and ends with a normal-metallic Fermi-liquid. The temperature below which superconductivity occurs reaches its maximum, $T_{c\ max}$, at a doping of ~0.15 holes per Cu and varies greatly with the material, from 0 to 150 K. The basic band structure, i.e. that of the Fermi liquid, has a less-than-half-full conduction band, dispersing predominantly in the *x* and *y*-directions and of character Cu $3d_{x2-y2}$ antibonding w3ith O $2p_{\sigma}$. The electron-electron correlations are significant in the underdoped (≤15%) phases, which are traditionally considered doped Mott-insulators. Their magnetic fluctuations are, however, coherent for sufficiently long length and times to enable the observation of quantum oscillations in the normal state stabilized by a high magnetic field, These oscillations are consistent with cyclotron orbits on a small Fermi surface reconstructed from the large Fermi surface given by standard local density-functional calculations and observed in overdoped materials by quantum oscillations and angle-resolved photoemission. The reconstruction gaps the flat, nesting parts of the large Fermi surface and leaves behind the curved parts. Those are the parts where, in the *d*-wave superconducting state, the gaps are respectively the largest and the smallest, the so-called anti-nodal and nodal directions. The mechanism of the superconductivity has not been understood, but presumably, the *d*-wave pairing is mediated by spin-fluctuations. Empirically, $T_{c\ max}$ is higher for materials with the large Fermi surface turned such that the flat parts are perpendicular to the *x*- and *y*-, rather than the *x*±*y* directions, equivalently, with the ratio of hopping between second and first-nearest neighbors, *t'/t*, being relatively large. This is achieved when the CuOє octahedral are strongly elongated along *z* and the covalency is large between apical oxygen and the cation counter to Cu.

Bulk nickelates are almost-cubic perovskites, because with configuration $3d^7$ not only ¾ of the antibonding d_{x2-y2}, but also of the antibonding $d3_{x2-1}$ orbitals are empty. $LaNiO_3$ is a paramagnetic, mass-enhanced metal. The Fermi surface hast two sheets, a large hole sheet centered at the corners of the Brillouin zone and a central, small electron sheet. They touch each other at the eight k-points equivalent with $\frac{1}{2}q_{111}$, where $q_{111} = \frac{2\pi}{a}(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. Along the cubic directions, the electron sheet extends a bit further, namely to about $0.42\frac{\pi}{a}$. For a constant k_x near the zone boundary, $\frac{\pi}{a}$, the cross-section is dx^2-y^2-like and resembles the Fermi-surface of the cuprates with the highest $T_{c\ max}$, whereas for smaller k_x, the cross-section becomes even more square. For k_z <0.42 $\frac{\pi}{a}$, it cuts not only the hole sheet, but also the electron sheet with which the cross-section is d_{3x^2-1}-like. Now, for a *single* layer of $LaNiO_3$, sandwiched between layers of an ideal, insulating, lattice matched oxide which makes the distance from Ni to its apical oxygens $\frac{a}{2}$, the bare band structure is approximately the build band structure with $_z$ fixed at the value $\frac{\pi}{2a}$, placing the nodes of the Bloch function at the apical oxygens. The actual value depends on the confining insulator and may thus be controlled. For a double layer the bare band structure is like that of the bulk for the two k_z values: $\frac{\pi}{2a}$ and $\frac{\pi}{4a}$, and so on. Hence,

confinement along *z* forbids the lowest k_z values and thereby rises the bottom of the d_{x^2-1} band, but leaves the d_{x2-y2} band unchanged.
As it became possible to build high-quality oxide heterostructures one atomic layer after the other by pulsed laser deposition or molecular beam epitaxy, it was suggested that, perhaps, one could make high-temperature superconductors by suitably confining nickelate monolayers, e.g. $LaNiO_3/n(DyScO_3)$. This has not come through, so-far. Found were instead, metallic or insulating magnetic phases which could be controlled by layer thickness and strain and thus potentially useful for devices. These phases resemble the insulating and magnetic phase of bulk nickelates with cations slightly smaller than La, specifically $PrNiO_3$ and $NdNiO_3$, for $T < T_N = T_{MI.}$ I shall describe them as double spin-spirals with the same wavevector q = q_{111} on the two fcc-like sublattices, but with different spin-moments, spin-directions, and charges. They occur as the result of nesting and the on-site electron-electron repulsion $U - 3J$. Complete moment disproportionation corresponds to singlet-triplet disproportionation and is what traditionally has been called charge disproportionation ($2d^7 \longrightarrow a^6 + d^8$), which is actually very small. With less than complete moment disproportionation, the magnetic structure is non-collinear. This last topic will be the main substance of the talk.

Martin Caffrey (Trinity College Dublin, Dublin)

In meso in situ serial femtosecond crystallography of membrane (and soluble) proteins

The lipid-based bicontinuous cubic mesophase is a nanoporous membrane mimetic with wide ranging applications in areas that include medicine, personal care products, foods, and the basic sciences. An application of particular note concerns it use as a medium in which to grow crystals ofmembrane proteins for structure determination by X-ray crystallography [1]. At least two variations of the mesophase exist. One is the highly viscous and sticky cubic phase which has well developed long-range order. The other, referred to as the sponge phase, is considerably more fluid and lacks long-range order. The sponge phase has been shown to be a convenient vehicle for delivering microcrystals of membrane proteins for serial femtosecond crystallography (SFX) at the Linac Coherent Light Source, SLAC National Accelerator Laboratory [2]. Unfortunately, the sponge phase approach calls for large amounts of protein which are not always available in the case of membrane proteins. The cubic phase offers the advantage of requiring significantly less protein for SFX [3-5] but comes with its own challenges. In this talk, I will describe the physico-chemical bases for these challenges, solutions to them and prospects for future uses of lipid mesophases for structure-function characterization of membrane and soluble proteins in the serial crystallography arena.

References

*[1] Caffrey, M., Li, D., Dukkupati, A. Membrane protein structuredetermination using crystallography and lipidic mesophases: Recent advances and successes. Biochemistry *51*: 6266, (2012)*

*[2] Johansson, L. C., *et al*. Lipidic phase membrane protein serial femtosecond crystallography. Nat. Meth. *9*:293, (2012)*

*[3] Liu, W., *et al*., Serial femtosecond crystallography of Gprotein-coupled receptors. Science *342*:1521, (2013)*

*[4] Weierstall, U., et al., Lipidic cubic phase injector facilitates membrane protein serial femtosecond crystallography. Nat. Commun. *5*:3309,(2014)*

*[5] Caffrey, M., Li, D., Howe, N., Syed S.T.A. 'Hit and run' serial femtosecond crystallography of a membrane kinase in the lipid cubic phase. Phil. Trans. R. Soc. B. *369*: 20130621, (2014)*

Majed Chergui (École polytechnique fédérale de Lausanne, Lausanne)

Tracking the electron in molecular systems and solid materials

"Photoinduced electron transport plays a crucial role in chemical, biochemical and condensed matter systems. The identification of the channel and final destination of the electron and the time scale of its transport require tools that provide elemental specificity with a high time resolution. I will illustrate how a combination of techniques: ultrafast optical visible spectroscopy, multidimensional UV spectroscopy and X-ray spectroscopies, can help identify electron dynamics in as diverse processes as electron transfer to the solvent in aqueous solutions, intraprotein electron transfer and electron injection and trapping in metal oxides. These examples will be discussed in the light of present models".

Tilman Esslinger (Eidgenössische Technische Hochschule Zürich, Zürich)

Bands with a twist and quantum sized steps

We use fermionic quantum gases to study the topological Haldane model in an optical lattice and the quantized conductance in an optically engineered quantum point contact for atoms. The Haldane model on the honeycomb lattice features topologically distinct phases of matter and describes a mechanism through which a quantum Hall effect can appear as an intrinsic property of a band-structure, rather than being caused by an external magnetic field. In our experiment we have realized the Haldane model in a periodically modulated honeycomb lattice and characterized its topological band-structure. Our approach allows for dynamically tuning topological properties and is even suitable for interacting fermions. In transport experiments the quantum nature of matter becomes directly evident when changes in conductance occur only in discrete steps, with a size determined solely by Planck's constant h. I will report on our observation of quantized conductance in the transport of neutral atoms.
This fundamental phenomenon has so far not been observed with neutral matter. In our isolated atom device we enter a regime in which the mean free path is larger than the system size.

Dmitri Golberg (Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan)

Nanomaterial Properties as Revealed by in-situ *Transmission Electron Microscopy*

Since recently *in-situ* transmission electron microscopy (TEM) has become a new powerful tool for the explicit analysis of electrical, mechanical, thermal and optical properties of diverse nanomaterials, *e.g.* nanotubes, nanowires, nanoparticles and "graphene-like" nanosheets. This method combines the highest spatial resolution peculiar to a high-resolution TEM instrument and unique possibilities of precise manipulations with an individual nanostructure, including its electrical biasing, Joule heating, charging, bending, stretching, peeling, and illuminating with a light of various wavelengths under a continuous control of all electromechanical and optoelectronic parameters.[1]

I will present our main progresses in regards of detailed studies of numerous, synthesized by us inorganic nanomaterials using a variety of *in-situ* "Nanofactory Instruments" TEM holders. Bending

and tensile strength, Young's modulus of carbon, boron nitride, and dichalcogenide nanotubes and nanosheets, silicon and boron nanowires and their peculiar deformation kinetics have been revealed under delicate mechanical tests. Ultimate increase in the nanostructure temperature up to ~2000^{o}C or more, using resistive heating have allowed us to shed a new light onto intra-diffusion and crystallization kinetics in the nanospace. Pioneering *in-situ* TEM optoelectronic tests on titanium dioxide nanoparticles, zinc oxide and silicon nanowires, cadmium sulfide nanobelts, molybdenum disulfide nanosheets and newly fabricated nanomaterial heterojunctions have led to clear understanding of their real technological prospects with respect to novel optoelectronic and photovoltaic device applications (Figure 1).

The author is extremely grateful to many colleagues: Drs. Daiming Tang, Zhi Xu, Mingsheng Wang, Xianlong Wei, Pedro Costa, Naoyuki Kawamoto, Masanori Mitome, Yoshio Bando, Ms. Maho Yamaguchi and Mr. Chao Zhang for taking part in the state-of-the-art experiments at different stages of the *in-situ* TEM Project accomplishment at MANA-NIMS over the last decades.

References:
1) D. Golberg *et al*., Adv. Mater. 24, 177 (2012).

Keywords: *in-situ* transmission electron microscopy, electrical properties, mechanical properties, optical properties, nanotubes, nanowires, nanosheets

Thierry Giamarchi (Université de Genève, Genève)

Local quenches and mobile impurities in cold atomic gases

Cold atomic systems have opened the possibility to study rapidly varying phenomena, such as a global or a local quench, in isolated quantum systems. One very interesting class of such phenomena is given by an impurity which is brutally released in a bath of other atoms. This situation occurs also naturally when atoms with different internal degrees of freedom ("spin") exist and is thus intimately related to the physics of propagation of "magnetic" excitations in such systems.
In the context of one dimensional systems the interactions between particles play an especially important role and give special properties to the bath. The physics of the impurity is strongly affected in such bathes and this leads, in addition to the standard polaronic renormalization of the impurity mass to behaviors such as subdiffusion via orthogonality catastrophy mechanisms.
I will discuss this physics and the analytical and numerical attacks to this problem. The theoretical results will be compared to the recent experiments that have been performed in cold atomic systems to test for such effects.

Thomas Irving (Illinois Institute of Technology, Chicago)

Time-Resolved Diffraction and Scattering from Non-Crystalline Biological Materials: Present Status and Future Prospects

One of the tenets of modern biology is that "structure of macromolecules determines function". Biological macromolecules frequently perform their function via large-scale structural changes on various time-scales. This talk will review the co-development of synchrotron sources and diffraction

and scattering techniques showing how technological innovations have enabled exciting new science. The current state of the art will be illustrated with examples of recent work in this area. The impact of new sources, including major upgrades to third generation synchrotron sources and 4th generation sources such as XFEL's will be discussed.

Patanjali Kambhampati (McGill Universtiy, Montreal, Canada)

Excitons in Semiconductior Quantum Dots: Design principles for lasers, optical switches, and LEDs

The semiconductor quantum dot is one of the canonical systems in nanoscience. Whereas the nanometer size of these materials is obvious, the richer and more meaningful issue is the presence of quantum confinement effects conferred by virtue of size. One may qualitatively describe quantum dot electronic structure like the textbook particle in a sphere. However, this simple picture misses the vast majority of the processes which ultimately control the functionality of the quantum dot. Our goal is to obtain a detailed picture of the rich inner workings of the quantum dot. We recently introduced a mixed time/frequency domain ultrafast spectroscopic approach which we denote *State-Resolved Exciton Dynamics*. We have applied this approach to both resolving long standing controversies as well as revealing new processes, including:

1) Hot exciton relaxation dynamics: *radiationless transitions on the nanoscale*
2) Optical gain: *recovering predictions from theory and revealing new physics*
3) Electronic structure of multiexcitons: *a platform for ultrafast all-optical logic*
4) Understanding the surface of quantum dots: *a path towards quantum dot LEDs*

Our newer work extends these efforts based upon our new developments in fully automated coherent 2D electronic spectroscopy, featuring complete polarization shaping of femtosecond pulses. With this approach, we are able to produce the first demonstration of ultrafast all-optical switching in quantum dots as a first step towards optical logic.

For more information, please visit: http://kambhampati-group.mcgill.ca/ and recent review articles:

1) “Unraveling the structure and dynamics of excitons in semiconductor quantum dots”, *Acc. Chem. Res.*, **44**, 1 (2011).
2) “Hot Exciton Relaxation Dynamics in Semiconductor Quantum dots: Radiationless Transitions on the Nanoscale”, *J. Phys. Chem. C*, **115**, 22809 (2011).
3) “Multiexcitons in semiconductor nanocrystals: A platform for optoelectronics at high carrier concentration”, *J. Phys. Chem. Lett*, **3**, 1182 (2012).

Cristiane Morais Smith (Utrecht University, Utrecht)

Engineering quantum states of matter in cond-mat and cold-atom systems

The recent realization of "synthetic graphene" by the self-assembling of semiconducting nano-crystals into a honeycomb lattice has opened new
perspectives into the realization of topological materials in condensed matter because Dirac cones were shown to occur in higher bands [1]. By choosing the chemical elements in the nanocrystal, the spin-orbit coupling can be tuned to a great extent, thus allowing us to engineer new materials that

could be useful for technological applications. A honeycomb lattice made of CdSe nanocrystals was shown to exhibit Dirac cones in the s and p conduction bands, as well as a topological phase in the *valence* band [1], whereas a honeycomb lattice of HgTe nanocrystals is prone to the realization of the integer and fractional quantum spin Hall effect in the c*onduction* band, protected by huge gaps [2].

Topological states of matter are being studied not only in condensed matter, but also in quantum optics. By loading ultracold fermions or bosons into optical lattices, it is possible to simulate cond-mat systems, thus custom tailoring model Hamiltonians which are supposed to describe complex quantum systems. The recent experimental realization of a p_x + i p_y Bose-Einstein condensate of Rb in a 2D optical lattice, for which time-reversal symmetry is spontaneously broken, is a nice example of the numerous possibilities to be explored with those systems [3]. A second compelling example of how cold atoms can be used as cond-mat simulators is provided by the investigation of phase coherence of a Rb BEC upon deformations of a 2D optical lattice. This system may shed some light into the destruction of superconductivity in high-Tc cuprates doped with rare earth atoms, such as Nd [4].

[1] E. Kalesaki, C. Delerue, C. Morais Smith, W. Beugeling, G. Allen, and D. Vanmaekelbergh, PRX 4, 011010 (2014).

[2] W. Beugeling, E. Kalesaki, C. Delerue, Y.-M. Niquet, D. Vanmaekelbergh, and C. Morais Smith, under review in Nat. Comm. (2014).

[3] M. Ölschläger, T. Kock, G. Wirth, A. Ewerbeck, C. Morais Smith and A Hemmerich, New Journal Phys.15, 083041 (2013).

[4] Marco Di Liberto, T. Comparin, T. Kock, M. Oelschlaeger, A. Hemmerich, and C. Morais Smith, Nat. Comm, in press (2014).

Matthias Weidemüller (Ruprecht-Karls-Universität, Heidelberg)

Simulating dipolar energy transport with giant atoms

Energy transport is an important theme in natural processes, e.g., chemical reactions and photosynthesis. There is ongoing debate on how the environment influences the efficiency of energy transfer in these systems and to which extent quantum mechanics plays a role. By interfacing electronically highly excited (Rydberg) atoms with laser light we simulate energy transfer dynamics in a controlled many-body system. In particular, Rydberg atoms experience quantum state changing interactions similar to Förster processes in complex molecules, offering a model system to study the nature of dipole-mediated energy transport. The extension to multiple interacting excitations could enable elementary realisations of quantum spin models involving strong and long-range spin-dependent interactions. We report on a new imaging method, which we apply to monitor the migration of electronic excitations with high time and spatial resolution using a background atomic gas as an amplifier. Through precise control of interactions and the coupling to the environment via the laser fields, we find different mechanisms at work which shed new light on the nature of energy and spin transport in complex quantum systems.