Prize Talk PRV I Mon 13:15 HSZ 01

Quantum Dots for Quantum Technologies — •Dieter Bimberg — TU Berlin and CIOMP of CAS Changchun — Laureate of the Stern Gerlach Medal 2020

Universal self-organization at surfaces of semiconductors lead to the formation of coherent quantum dots (QDs). Their electronic and optical properties are close to those of atoms in a dielectric cage. Their delta-function density of states is only twofold degenerate [1]. All few particle states are strongly Coulomb-correlated due to the strong carrier localisation. Their energies depend on shape and size of the dots, such that positive, zero or negative biexciton binding energies and fine-structure splitting appear [2].

Applications of single, few and millions of QDs for novel Quantum Technologies will be demonstrated.

a. Single QDs can be emitters of Q-bits on demand or entangled photons for future quantum security systems. In electrically pumped RCLED structures, emission of q-bits at rates beyond 1 Gbit/s were shown [3, 4].

b. Hybridization of Flash and DRAMs, bringing together the advantages of both types of memories, is the "Holy Grail" of memories and ensures future memory development after the end of Moore's law. The goal of non-volatility (i.e. storage time $>$ 10 years) can be achieved for the storage of holes in type II (InGa)Sb QDs embedded in a (AlGa)P matrix [5].

c. The demand for higher data rates in optical networks, requires novel ultra-high bit rate energy efficient sources. QD Lasers based on GaAs emit up to the O-band at 1.3 μm, showing record low jth and complete temperature stability up to 80°C. Passive mode-locking generates pulses in the sub-ps range at repetition rates up to 90 GHz. The hat spectrum of one single laser of several tens of closely spaced narrow lines is thus a potential pulse source for bit rates up to $\approx$ 6 TBit/s using DQPSK [6].

[1] M. Grundmann, O. Stier, D. Bimberg, *Pyramidal Quantum Dots – Strain Distribution, Optical Phonons, and Electronic Structure*, Phys. Rev. B **52**, 11969 (1995); O. Stier, M. Grundmann, D. Bimberg, *Electronic and optical properties of strained quantum dots modelled by 8-band k.p theory*, Phys. Rev. B **59**, 5688 (1999)

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[3] A. Schliwa, M. Winkelnkemper, A. Lochmann, E. Stock, D. Bimberg, *(InGa)As/GaAs quantum dots grown on a (111) surface as ideal sources of entangled photon pairs*, Phys. Rev. B **80**, 601307(R) (2009)

[4] W. Unrau, D. Bimberg, *Flying q-bits and entangled photons*, Laser Photonics Review **8**, 276 (Wiley, 2014)

[5] L. Bonato, F. I. Arikan, L. Desplanque, C. Coignon, X. Wallart, Yi Wang, P. Ruterana, D. Bimberg, *Hole Localization Energy of 1.18 eV in GaSb quantum dots embedded in GaP*, Phys. Stat. Sol (b) **10**, 1877 (2016)

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Prize Talk PRV II Mon 15:00 WIL B321

Hartree-Fock simulation of hematite surfaces with *a posteriori* calculation of correlation energy — •David Scholz[1,2] and Thomas Stirner[1] — [1]Technische Hochschule Deggendorf, 94469 Deggendorf, Germany — [2]Laureate of the Georg Simon Ohm Prize 2020

Hematite (α-Fe_2O_3) is from a technological and scientific viewpoint very interesting, in particular as catalyst, for the electro-chemical splitting of water, as magnetic sensor and as anode material for lithium-ion-batteries. Furthermore it exhibits strong correlations due to its localized 3d-electrons. In this bachelor thesis different crystalline surfaces of hematite were investigated by computer simulation via the Hartree-Fock method and an *a posteriori* calculation of the correlation energy. The surface energy and structure were calculated for each surface and compared in order to find the most stable facets of hematite. This talk presents the results of the bachelor thesis. On the example of the (001)-surface the influence of the electron correlation on the surface energy is demonstrated. For comparison the surface energy of chromia (α-Cr_2O_3) and alumina (α-Al_2O_3) are also shown. The calculated surface relaxations of hematite are compared with results from experiments and density functional theory.

Prize Talk PRV III Tue 13:15 HSZ 01

Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain — •Zhe Wang — Institute of Physics II, University of Cologne, Cologne, Germany — Laureate of the Walter Schottky Prize 2020

One-dimensional (1D) spin chains are text-book examples for illustrating basic concepts, such as phase transitions and spin dynamics. Apart from magnon excitations with an integer quantum number, excitations with fractional quantum number (e.g. spinons with S = 1/2) and complex magnon bound states (i.e. Bethe strings) are usually introduced also in the context of spin-chain models. As being exactly solvable, the 1D models provide understanding of the basic concepts in an exact sense, thus it is also a subject of a constant stream of theoretical studies. However, an experimental study of the exotic magnetic excitations is far from straightforward. This is because a proper material realization of the 1D models is scarce, and the magnetic excitations need to be disentangled from other degrees of freedom and at the same time, detectable by available experimental techniques. Recently, these difficulties are overcome in our experimental studies of the spin-1/2 antiferromagnetic Heisenberg-Ising chain compounds SrCo2V2O8 and BaCo2V2O8. I will present our terahertz spectroscopic investigations of quantum spin dynamics in these compounds as a function of temperature and high magnetic fields. In particular, we have been able to identify the long sought-after many-body string excitations, the excitations of confined spinons, as well as magnons, which are characteristic for the different phases connected by magnetic field-induced quantum phase transitions in the 1D spin-1/2 Heisenberg-Ising antiferromagnet.

Prize Talk PRV IV Wed 13:15 HSZ 01

Fingerprints of correlation in electronic spectra of materials — •Lucia Reining — Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA/DRF/IRAMIS, Institut Polytechnique de Paris, F-91128 Palaiseau, France — European Theoretical Spectroscopy Facility (ETSF) — Laureate of the Gentner Kastler Prize 2020

Many properties of materials are determined by electronic excitations which can be observed in spectroscopic experiments, such as absorption or photoemission. However, electronic spectra of a real many-body system are often very different from what an independent-particle picture would suggest. How can theory understand, and how can calculations predict, the wealth of unexpected phenomena that may take place ? Density functional theory and many-body perturbation theory based on Green's functions are powerful approaches to face this problem, and indeed, ab initio calculations often yield reliable band structures. However, electronic excitation spectra contain much more: they may exhibit lifetime broadening, an incoherent background or distinct satellite structures. These features are pure correlation effects that cannot be captured by any independent-particle picture, and they are at the forefront of the capabilities of current first principles approaches. In this talk we will discuss recent progress in the theoretical description and analysis of satellites in photoemission and inelastic x-ray scattering spectra, using density functionals [1], Green's functions [2], and close collaboration with experiment. [1] M. Panholzer, M. Gatti, and L. Reining, Phys. Rev. Lett. 120, 166402 (2018). [2] J.S. Zhou, et al., J. Chem. Phys. 143, 184109 (2015); Phys. Rev. B 97, 035137 (2018).

Prize Talk PRV V Wed 15:00 WIL A317

Toward Atomic-Scale Optical Spectroscopy in Plasmonic STM Junctions — •Takashi Kumagai — Fritz-Haber Institute of the Max-Planck Society — Laureate of the Gaede Prize 2020

Light-matter interactions can be largely enhanced in the presence of optical near fields. Atomic-scale light-matter interactions in plasmonic 'picocavities' has emerged as a new frontier of fundamental physics [1]. The investigation of such light-matter interactions involves significant challenges for both experiment and theory. A combination of plasmon-enhanced spectroscopy with low-temperature STM can provide a unique way to investigate intriguing physics resulting from the strong interaction between cavity-mode plasmon and matter. I will show our recent development toward atomic-scale optical spectroscopy in plasmoic STM junctions [2-5]. References: [1] Science 354, 726 (2016). [2] PRL 121, 226802 (2018). [3] J. Phys. Chem. Lett 10, 2068 (2019). [4] Nano Lett. 19, 3597 (2019). [5] Nano Lett. 19, 5725 (2019).

Prize Talk PRV VI Thu 13:15 HSZ 02

Charge-state controlled imaging of electronic transitions in single molecules — •Laerte Patera — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — Laureate of the Gustav Hertz Prize 2020

Electron transfer plays a crucial role in many chemical processes, from

photosynthesis to combustion and corrosion. However, the way in which redox reactions affect individual molecules and, in particular, their electronic structure, remains largely unclear. Unveiling these fundamental aspects requires the development of experimental tools allowing the observation of electron transfer down to the single molecule level. In my talk, I will present an innovative experimental approach capable of performing tunneling experiments on non-conductive substrates, to map the orbital structure of isolated molecules upon electron transfer. By driving a change in the redox state of a molecule synchronized with the oscillating tip of an Atomic Force Microscope, previously inaccessible electronic transitions are resolved in space and energy [1]. These results unveil the effects of electron transfer and polaron formation on the single-orbital scale, opening the door to the investigation of redox reactions and charging-related phenomena with sub-Ångström resolution.

[1] L. L. Patera, F. Queck, P. Scheuerer and J. Repp, Nature 566, 245-248 (2019)