大阪大学 OSAKA UNIVERSITY

rijksuniversiteit groningen

INSD NanoScience Video Exchange Lectures (2024, Groningen-Osaka)

These lectures are held as a part of **"Fundamental and functional properties of nanomaterials"** in top Master NanoScience in Groningen and as **"International Exchange Lectures on Nanoscience and Nanotechnology A"** in INSD Nano Program in Osaka. The program is also shared by University of Science-Malaysia, King Mongkut's Institute of Technology Ladkrabang-Thailand, and Institute for Materials Science VAST-Vietnam.
The lectures except for October 11th start on the following Fridays at 9:00 in the morning (Groningen time), that is, at 16:00 or 17:00 in the afternoon (Osaka time).
[NOTE The Netherlands switches from summer time (day light saving time) to winter time on the night of October 27th (Sun) 01:00 (UTC) 2024.]

Lecture 0

Friday, 11 Oct. 2024
Osaka time: 16:00-18:15 (no exchange lecture from Groningen)

Prof. Tadashi Itoh, Institute for NanoScience Design (speaks 16:00-18:15 (O))
(Field: solid state physics, semiconductor nanocrystal (quantum dot), optical properties)
Title: Introduction, Photophysics of quantum dots.
(Together with video address and Nobel-Prize lecture given by Prof. Benard L. Feringa)
Abstract: Electronic excited states (excitons) in semiconductor nanocrystals show peculiar quantum size effects which exhibit various kinds of characteristic optical properties; blue shift and splitting of the exciton energy states, rapid radiative decay, ultrahigh speed giant optical nonlinearity, highly efficient lasing, etc.
The video address and the Nobel Prize Lecture given by UG Prof. Benard L. Feringa will follow.

Lecture 1

Friday, 18 Oct. 2024
Osaka time: 16:00-18:00
Groningen time: 9:00-11:00

Chair: Prof. Loredana Protesescu
Prof. Antonia Gubisic-Cabo (9:00-9:55 (G) / 16:00-16:55 (O))
Title: Kinetic *In situ Single-layer* Synthesis (KISS) technique for large-area 2D materials exfoliation:
Abstract: Two-dimensional (2D) materials offer a remarkably rich platform for exploring novel quantum phenomena and designing nanostructures with tailored functionalities. Since 2D materials consist almost entirely of a surface, the field of surface science is central to their investigation. This field is broad and diverse, encompassing studies of structural changes on surfaces, the development of growth methods for 2D materials, and the exploration of their electronic properties using techniques such as angle-resolved photoemission spectroscopy (ARPES).

In my research group, we focus on all these aspects, with particular emphasis on the electronic structure. We use ARPES and time-resolved ARPES, which provide direct images of a material's electronic structure, to study how it evolves as materials are thinned from 3D to 2D, or when

different substrates are used. We also investigate ways to manipulate electronic properties either statically (with ARPES) or dynamically (with time-resolved ARPES), by tuning the electronic structure or altering its topology.

In today's lecture, I will introduce a novel method for the *in situ* exfoliation of 2D materials, performed directly in ultra-high vacuum (UHV). This approach produces large flakes with excellent crystallinity and purity. In our experiments, we successfully exfoliated various semiconducting and metallic transition metal dichalcogenides onto substrates like Au, Ag, and Ge, demonstrating the versatility of this technique, which was then characterized using ARPES.

This method is not only straightforward and simple, but also requires no specialized equipment. It is particularly well-suited for investigating the electronic structure of air-sensitive 2D materials, as the entire sample preparation occurs within an UHV environment.

Chair: Prof. Yoshikata Nakajima

Prof. Hidekazu Tanaka, SANKEN (Institute of Scientific and Industrial Research)

(17:00-17:55 (O) /10:00-10:55(G))

(Field: electronic/magnetic/optical properties of oxide thin films and their nanostructures)

Title: Basics and applications of electronic phase change oxides

Abstract: Phase change materials enable rapid switching between different structural phases, resulting electric properties switching. Some classes of materials are interesting on switching between different electronic/spin phases itself, such as Mott insulator-metal transition, and their electronic phase change would produce new classes of devices. This part of the lecture will focus on electronic phase change phenomena on transition metal oxides. Following topics will be included, ・Physics and material science on structural and metal/insulator transition, ・Brief review of phase change phenomena on transition metal oxides (vanadate, manganite, nickelate, ferrite, ruthenate, etc.), ・External field induced electronic phase change phenomena, ・Oxide Iontronic, ・Switching/Memristive /Biology-inspired /Photonic devices based on electronic phase change materials.

Lecture 2

Friday, 25 Oct. 2024

Osaka time: 16:00-18:00

Groningen time: 9:00-11:00

Chair: Prof. Yoshikata Nakajima

Prof. Yoshitada Morikawa, Graduate School of Engineering (16:00-16:55 (O) /9:00-9:55(G))

(Field: computational science, surface science, DFT, machine learning, CO_2 hydrogenation)

Title: Computational Materials Design for Surfaces

Abstract: Chemical reactions at surfaces and interfaces play important roles in wide ranges of applications such as heterogeneous catalysis, electrochemistry, fuel cells, batteries, etching processes of semiconductor materials, and so on. In this lecture, I will present density functional theory (DFT) investigation and prediction of hydrogenation of CO_2 over Cu catalyst. To clarify reaction mechanisms and to identify important factors governing the reactivity of CO_2 on solid surfaces are very important to develop more efficient catalysts or catalytic processes for utilization of CO_2. Although DFT simulations are quite useful to investigate atomic-scale phenomena, the time scale of the simulations is limited to tens of ps and the length scale to nm. I will discuss how to extend the length-scale and time-scale of DFT simulations by combining DFT calculations with machine learning techniques. I will show that it is now possible to clarify the formation process of Cu–Zn surface alloy, which has been extensively studied for the clarification of the true active site of $Cu/ZnO/Al_2O_3$, the industrial catalyst for methanol synthesis which remains under controversy.

Chair: Prof. Loredana Protesescu
Prof. Erika Covi (10:00-10:55 (G) / 17:00-17:55 (O))
Title: Memristive and CMOS Technologies for Advanced Cognitive Systems
Abstract: In the past two decades, the shift towards a distributed computing paradigm led our smart systems to become more and more interconnected. These systems need to elaborate increasingly amount of data while featuring low-power operation, area efficiency, and ability to interact with the external world in real time. Memristive technology, with its unique characteristics and capabilities, holds great promise for the design of such cognitive systems. The potential for energy-efficient and parallel computing, combined with the ability to integrate complex neural and synaptic dynamics within a single device, provides avenues for high-performance hardware implementations. Moreover, by offering volatile and non-volatile memory in a small footprint, enabling dense integration, and facilitating in-memory computing, memristive technology presents advantages that, if correctly combined with CMOS technology, can extend the functionality of current artificial intelligent systems.

In this talk, we discuss the challenges and the opportunities to realise memristive neuromorphic computing by developing novel hardware architectures and learning algorithms specifically tailored to best exploit the intrinsic properties of memristive technology. Indeed, we show that memristive technology offers vast potential, but its effective utilization relies on the synergetic development of memristive devices, circuits, and algorithms to create performing hardware cognitive systems.

Lecture 3

Friday, 8 Nov. 2024

Osaka time: 17:00-19:00
Groningen time: 9:00-11:00 (in winter time)

Chair: Prof. Yoshikata Nakajima
Prof. Hiroshi Miyasaka, R3 Institute for Newly-Emerging Science Design
(17:00-17:55 (O) / 9:00-9:55(G))
(Fields: Photochemistry in condensed phase and ultrafast detection of chemical reactions)
Title: Photochemistry with multiphoton absorption and multiple excitation in the condensed phase
Abstract: Molecules in the electronic excited state take important roles in various photo-functional systems. Multiphoton absorption and multiple excitation are one of methods to explore photochemical reactions beyond conventional limitations in molecular photochemistry in the condensed phase. In this lecture, we will introduce the background of the conventional photochemistry, multiphoton absorption & multiple excitation, and several examples of specific photochemical responses induced by these nonlinear absorption processes.

Chair: Prof. Loredana Protesescu
Prof. Jagoda Sławińska (10:00-10:55 (G) / 18:00-18:55 (O))
(Field: computational materials science, spintronics)
Title: Spin-orbit-related phenomena for energy-efficient electronic devices
Abstract: In this lecture, I will discuss the fundamentals of spintronics (spin-based electronics) which employs the electron's spin, along with its charge, to carry and process information in a more energy-efficient way. Spin-orbit interaction, despite being small in magnitude, is very powerful and drives several intriguing phenomena that allow for different functionalities suitable for novel electronic devices. After explaining the basic principles and challenges of spintronics, I will focus on materials for conversion between charge and spin currents and their computational design via first-principles calculations.

Lecture 4

Friday, 15 Nov. 2024

Osaka time: 17:00-19:00
Groningen time: 9:00-11:00 (in winter time)

Chair: Prof. Yoshikata Nakajima
Prof. Yasuhiro Nakazawa, Graduate School of Science (17:00-17:55 (O) /9:00-9:55(G))
(Field: Molecular superconductors, electron correlations, thermodynamics)
Title: Molecular superconductors and their thermodynamics
Abstract: The organic-molecules-based conductors and superconductors give a variety of physical features of itinerant π-electrons released from molecular orbitals. Fascinating physical and chemical features related to the electron correlations, electron-phonon interactions emerge in them with various manners, since the energy scale of spin, charge, and phonon degrees of freedom are in the similar order. The lecture focus on why the interesting conducting states, especially superconductivity with unconventional characters appear in them and how we can characterize the electronic properties by means of micro-crystal thermal measurements.

Chair: Prof. Loredana Protesescu
Prof. Jan Anton Koster (speaks 10:00-10:55 (G) / 18:00-18:55 (O))
Title: Perovskite solar cells: what can we learn from numerical modelling?
Abstract: Despite the rapid development of perovskite solar cells several challenges remain. A deeper understanding of the main losses, and how to mitigate them, is needed to make targeted improvements possible. In this talk, I will discuss two types of modelling techniques that shed new light on these fascinating solar cell materials.

Drift-diffusion techniques make it possible to connect and explain the fundamental generation, transport and extraction processes to macroscopic device performance. If done right, one can also do the opposite: By reverse-engineering current-voltage measurements on actual solar cells, one can identify the limiting factors. As an example, we show how current-voltage data and electroluminescence measurements help us identify the voltage losses in a series of co-evaporated FACsPbIBrCl perovskite solar cells with organic transport layers.
The hot carrier solar cell concept has been proposed to overcome the Shockley-Queisser limit, by harvesting carriers before they have lost their surplus energy. Perovskites how promise for this type of application as some perovskites have shown very long cooling times, the key requirement for a hot carrier solar cell.

By using an ensemble Monte Carlo (EMC) simulation we are able to simulate the trajectories of charge carriers and model their interactions with their environment. In EMC random free flight times are generated and interrupted by scattering events with desired scattering mechanisms. It is this freedom of choice which makes EMC an excellent tool in order to investigate what exactly causes charge carriers in halide perovskites to cool.

In this contribution we first identify the roles of electron-phonon and electron-electron scattering in the thermalisation and cooling process. We show how these processes depend on several material parameters. We zoom in on how cooling times are impacted by the degree of background doping and show how an ensemble of background carriers can have a detrimental effect on the cooling time. Next, we quantify the effect of a hot phonon bottleneck on the cooling time. The hot phonon bottleneck has been put forward as a prominent mechanism explaining the extended cooling times measured for perovskites. We show on what scale the hot phonon bottleneck could extend cooling times and how it depends on carrier concentration and phonon lifetime.