

Origin and structure of polar domains in doped molecular crystals*

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Doping is a primary tool for the modification of the properties of materials. Occlusion of guest molecules in crystals generally reduces their symmetry by the creation of polar domains, which engender polarization and pyroelectricity in the doped crystals. Here we describe a molecular-level determination of the structure of such polar domains, as created by low dopant concentrations (<0.5%). The approach comprises crystal engineering and pyroelectric measurements, together with dispersion-corrected density functional theory and classical molecular dynamics calculations of the doped crystals, using neutron diffraction data of the host at different temperatures. This approach is illustrated using centrosymmetric α -glycine crystals doped with minute amounts of different L-amino acids. The experimentally determined pyroelectric coefficients are explained by the structure and polarization calculations, thus providing strong support for the local and global understanding of how different dopants influence the properties of molecular crystals.

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Enhanced hydrogen production with chiral conductive polymer-based electrodes

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Abstract

Efficient photo-electrochemical production of hydrogen from water is the aim of many studies in recent decades.¹ The goal is to find an inexpensive catalyst that reduces the electric potential required to initiate the process.² It was suggested that by controlling the spins of the electrons that are transferred from the solution to the anode, and ensuring that they are co-aligned, the threshold voltage for the process can be decreased to that of the thermodynamic voltage.³ In the present study, chiral conductive polymer is used to obtain high current density, low overpotential, and by-product-free hydrogen production. Anodes coated with chiral conductive polymer result enhancement in hydrogen production from water and the threshold voltage is reduced, as compared with anodes coated with achiral polymer. When CdSe quantum dots were embedded within the polymer, the current density was doubled. These new results point to a possible new direction for producing inexpensive, environmental friendly, efficient water splitting photo-electrochemical cells.

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Coherent tunneling through azurin monolayers

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Abstract: CB is a phenomenon generally observed in single molecule measurements where the presence of an electron on a molecule prevents other electrons moving onto the molecule, thereby blocking the current through the molecule, no longer obeying Ohm's law. We measured electron transport across a redox active protein in a solid-state junction using Au (substrate)/protein//linker/ Au (top) tunnel junction configuration, with the Cu(II) redox centre of the electron transfer protein Azurin (Az) shielded from direct interaction with the Au (top) electrode, by a monolayer of (< 1 nm) linker molecules, bound covalently to the Au (top) electrode. In contrast to what is the case without such linker layer, the differential conductance of the current-voltage (I-V) characteristics observed at low temperatures (~6 K), shows clear steps and its first derivative a peak-like structure, rather than the earlier observed inelastic electron tunneling spectrum. Given the nature of the junction, the most likely cause for this result is the redox active protein, specifically its redox-active moiety, the Cu ion. The satellite peaks which are positioned at 50 meV away from the main peak indicates Cu-S stretching vibration peaks. The conductance peak shows clear temperature dependence, theoretical calculations carried out indicates resonant tunnelling through discrete energy levels, which serves as a definite proof that transport through azurin is coherent in nature. The non-linearities in the conductance can then be explained by charging of the Cu redox centre. This hypothesis was tested and verified by experiments with the Cu removed from the protein, yielding apo-Az.

Tuning Electronic Transport via Hepta-Alanine Peptides Junction by Tryptophan Doping

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Biomolecules display great potential for future functional molecular electronic devices. Peptides are suitable as building blocks to bridge conductive electrodes in solid state electronic devices. To design and apply peptide junctions for solid state devices, the relations of peptide electron transport to their amino acid composition and structure need to be understood as well as the peptide electronic structures on the electrode surface. Such information may also help understanding the electron transfer processes that occur in/with proteins in biological energy conversion, sensing and signaling systems.

Earlier we studied electron transport across self-assembled homopeptide monolayers of specific amino acids, length and structure, between gold contacts. Supported by high-level electronic structure calculations we found the nature of the amino acid, charge of its residue, length and secondary structure to determine the peptide conduction, which we suggested to be dominated by off-resonance tunneling¹.

We then used a series of heteropeptides, linear oligo-alanines with a single tryptophan substitution, which acts as “dopant”, introducing a low-lying energy level. Trp doping markedly increases peptide conductance, especially if its location in the sequence is close to an electrode. Combining inelastic tunneling spectroscopy (IETS), ultraviolet photoelectron spectroscopy (UPS), advanced density-functional theory (DFT) electronic structure calculations, and current-voltage analysis, the role of Trp in ETp is rationalized by tunneling across a heterogeneous energy barrier, due to Ala and Trp electronic states, and Trp coupling to the electrodes. These results reveal a controlled way of modulating the electrical properties of molecular junctions by tailor-made “building block” peptides².

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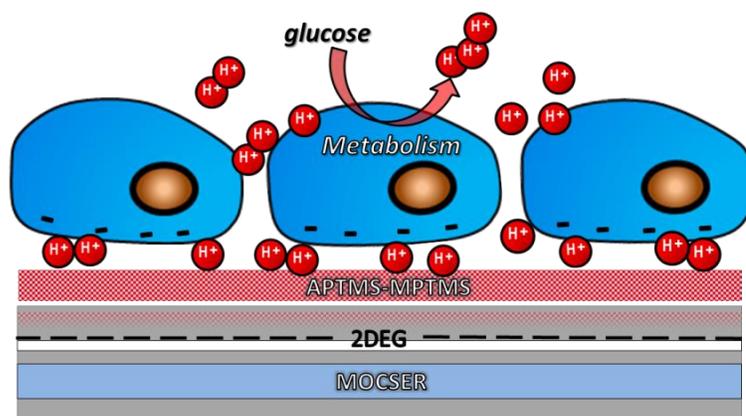
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Sensing cellular activity via the molecular controlled semiconductor resistor

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During the last decade we developed a GaAs based Molecular Controlled Semiconductor Resistor (MOCSER) device that was applied as a molecular sensor both in gas¹ phase and in solutions². Several properties of GaAs make it attractive for the development of biosensors, among others the high electron mobility and the ability to engineer the device properties by proper layer growing. We have managed to overcome its inherent chemical instability by developing a surface protecting layer, using a polymerized 3-mercaptopropyl-trimethoxysilane (MPTMS)³. In the current work we developed a biosensor for real time electronic label-free monitoring of cellular activity, using the MOCSER technology. In order to improve cell adhesion and biocompatibility, the MPTMS coated devices were modified with an additional layer of aminopropyl-trimethoxysilane (APTMS). HeLa cells were found to grow successfully on these devices. MOCSER devices cultured with these cells are stable and could sense cellular activity. HeLa cellular metabolic activity was tested at different glucose concentrations and showed a positive correlation to glucose concentration. We believe that this response is due to the high proximity between the cells and the device. The sensing mechanism of the MOCSER is mainly related to the occurrence of surface acidification, due to the release of protons by the cells. We propose to apply the coated MOCSER for real-time and continuous monitoring of cellular activity.



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Spin-dependent electrochemistry without magnet

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The chiral Induced Spin Selectivity (CISS) effect causes one spin orientation to be preferred when electrons are transported through chiral molecules.¹ This allows the magnetization of ferromagnetic film by spin torque transfer.² We report on novel technique in which spin selective electrochemistry is monitored via spin accumulation in an Hall type device³ that serves as the working electrode in the electrochemical cell. The strength and sign of the Hall signal correlates with the chirality and the length of the chiral molecules.

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Molecular Half Metallicity: extreme intramolecular spin filtering and magnetoresistance

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Perhaps the most essential requirement for spintronic manipulations is the generation of highly spin-polarised currents. This property is achieved in half metals that act as metals for one spin type and as insulators for the opposite spin. Half metallic compounds were first predicted and then found already two decades ago, however half metallicity was never demonstrated in nanoscale structures, despite the great promise for highly efficient nanoscale spin manipulations. Here, we show that half metallicity can be realized at the level of a single molecule in a molecular junction based on a molecular magnet suspended between two non-magnetic electrodes. The junction show over 90% spin filtering and 1-3 orders of magnitude magnetoresistance. The results are explained with the aid of DFT calculations and control experiments in the framework of spin splitting of energy levels and molecular anisotropic magnetoresistance.

Direct Metal to Halide Perovskite (HaP) Transformation an Alternative Route to HaP films

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We will present a simple process to convert a metallic film of $\text{Pb}^{(0)}$, $\text{Sn}^{(0)}$ or a mixture of those to an ABX_3 halide perovskite by introducing to AX [e.g.: A - methylammonium iodide (MAI), formamidinium (FA) or Cs; X - I, Br] salts dissolved in simple alcoholic solvents.[1] The novel approach allows a high-quality continuous films of various (including mixed) halide perovskites, that can be easily up-scaled to large areas using a low toxicity process. The much diminished toxicity of this fabrication method is achieved by avoiding the use of commonly used polar aprotic solvents, such as dimethylformamide or dimethylsulfoxide, which become very toxic when containing Pb salts (such as PbX_2 or Pb-acetate).

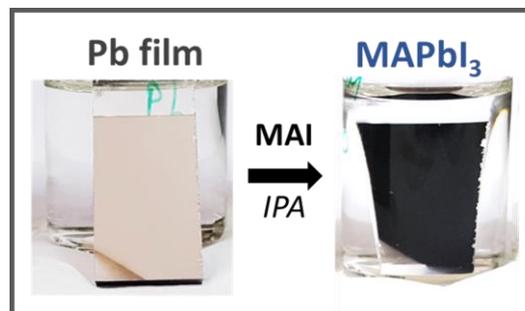


Figure: Pb film (~ 100 nm) evaporated on d-TiO₂ /FTO/glass substrate glass before and after treatment with MAI dissolved in IPA

We will describe of our findings, including examples of the direct transformation from Pb or Sn to, for example, MAPbI_3 , MAPbBr_3 , $\text{MAPb}(\text{Br},\text{I})_3$, MASnI_3 and the pseudo-perovskite Cs_2SnI_6 . We will show the broad morphological tunability allowed by this process and present how *electrochemistry* can further assist in optimization of the process. Apart from I-V characterizations of full devices, morphological, optical and (opto-)electronic characterizations will be presented.

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Shot noise on atomic and molecular junctions: extension to the MHz range

A single metallic atom or a molecule connected between two nanoelectrodes form the smallest electrical wires. Using Mechanically Controllable Break Junctions (MCBJ) we can produce such junctions and study the electronic transport. Analyzing the current flowing through the contact we observe fluctuations in the average current. These statistical fluctuations can be identified as the thermal noise due to the thermal excitation of the electrons and as shot noise due to the non-equilibrium occupation of the electrons under applied bias voltage.

Shot noise experiments give us information about the number of channels of transmission, providing in this way information about the nature of the binding. More recently we have shown that shot noise can also give information on the inelastic scattering processes at the atomic scale. In order to separate these effects from spurious $1/f$ noise we have developed an extension of the experiments from the previous range of 100kHz to a new limit of 10MHz, exploiting cryogenic amplifiers close to the junction. The experiments will help us understand the mechanism of dissipation in molecular electronic transport.

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Thermoelectric noise – beyond thermal and shot noise

Electronic current noise was proved to be a very useful tool for the study of electronic transport in nanoscale conductors. Up to now two fundamental types of current noise were identified: the electron thermal noise (Johnson–Nyquist noise) and shot noise (denoted as partition noise). The first is generated in equilibrium by finite temperature and the second by an applied voltage. Recently, we found indications for the generation of a new type of partition noise that is generated when a temperature gradient is applied across a nanoscale conductor. The temperature gradient breaks the symmetry of electronic transmission even in the absence of a voltage drop and has different properties in comparison to thermal or shot noise. While this “thermoelectric noise” is interesting from the fundamental point of view, it can serve as a useful temperature gradient probe, and should be taken into account when the size of electronic circuits approaches the miniaturization limit.

Ron Naaman - Methods for creative education

Irit Naaman, Oded Naaman, Adi Diner, Einat Sitbon

Creating curiosity in young minds, and inspiring both critical and creative thinking is a task most educators and parents struggle with.

Ron Naaman, both as father and as grandfather, used a multitude of everyday events to provoke creativity and independent thought.

The most minute events were employed for these purposes. Spilled juice was used as an example of entropy, as well as more structured explanations of electron spins, while children were spinning around the house.

Education is not only science, and indeed Ron's education of his children and grandchildren has included deep discussions regarding current events, as well as hiking trips around Israel and educational trips around the world. For example, a study was conducted regarding the best Ice cream , namely "Blue Ice" in Piazza Navona in Rome, and the best way to climb the Annapurna trail in Nepal.

We here present a description of methods to nurture such thinking, as recorded over several decades. The descriptions here are but examples of a lifetime of education, which is still ongoing.

Electronic transport in reduced graphene oxide prepared by different routes

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In order to exfoliate graphite to single layers, the well-established oxidation process of graphite is conducted at relatively high temperature (1). During high-temperature oxidation and reduction, a release of CO₂ molecules is observed causing an irreversible degradation of atomic structure of graphene. Recently, a low-temperature process of oxidation and reduction was developed [2]. We prepared graphene by both high-T and low-T processes and compare the resulting atomic structures of graphene flakes imaged by scanning transmission electron microscope (STEM); while the graphene flake prepared by the high-T process loses its long-range crystal order, the flake made at low-T preserves the long-range order very well.

For the electrical transport study graphene layers were made by filtrating suspensions of both graphene materials. Then temperature dependences of conductivity from room temperature down to 4.2 K were measured. We observe a significant difference in absolute values of several orders of magnitude as well as in transport mechanisms: for the high-T route made graphene variable range hopping model fits the experimental curve, for the well crystalline graphene made at low-T tunnelling mechanism fits the measurement better.

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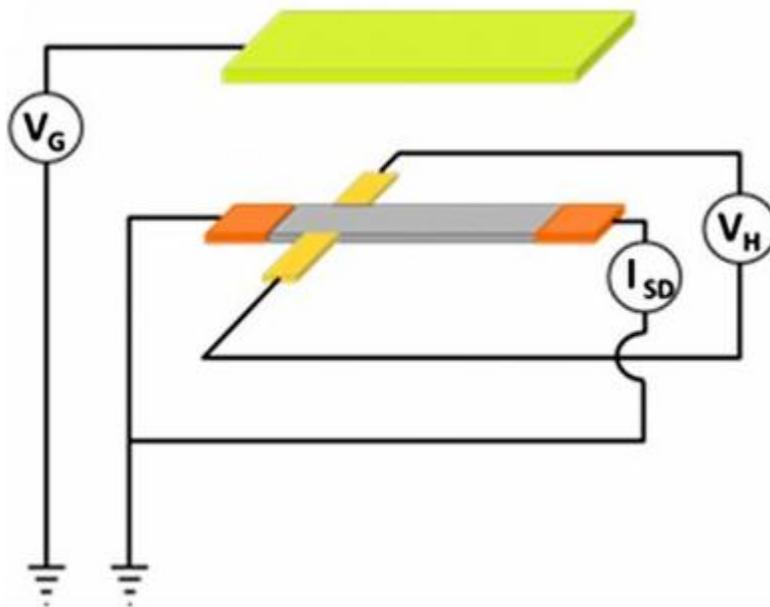
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Solid State Electric Hall Measurements of Chiral Monolayers

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The possibility to create spintronics devices with no magnetic materials have been proposed and realized^[1] in recent years, using the Chiral Induced Spin Selectivity effect (CISS). Using a magnet less Hall device it was shown^[2] that charge transfer through chiral monolayers magnetizes the substrate. Recently, similar achievement had been reached by applying only an electric dipole on the monolayer, using a buffer solution^[3].

In this research we use for the first time a solid state hall device to measure, at microsecond's time scale, the Hall signal generated by directly applying an electric dipole onto a chiral monolayer. Effective magnetic field of up to 100 gauss was measured for the first few microseconds.



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Towards Spin-Organic Light Emitting Diode (sOLED)

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The possibility to create spintronics devices with no magnetic materials have been proposed and realized^[1] in recent years, using the Chiral Induced Spin Selectivity effect (CISS)^[2]. Chiral polymers have drawn interest due to their potential to easily produce spin selective layers, applicable in spintronics and specifically in organic LEDs.

Theoretically, controlling the spin of the electrons and holes in OLEDs will quadruple their efficiency, and will cause the eminence of circularly polarized light.

In the current research the circular polarization of the electroluminescence and fluorescence of thin (~100 nm) layers of chiral F8BT (Poly[9,9-bis((S)-3,7-dimethyloctyl)fluorene-alt-benzothiadiazole])^[3] was studied at various annealing temperatures.

A strong dependence of the circular polarization on the annealing temperature was found in the polymer. While no circular polarization was measured without annealing, up to 13.5% (asymmetry factor $g=0.27$, figure 1) circular polarization of the electroluminescence was measured after annealing at 240C⁰, just below the melting point of the polymer. This suggests the source of the circular polarization is the formation of small chiral clusters, locally affecting the fluorescence of the polymer. The measured circular polarization of the fluorescence was consistently lower than the circular polarization of the electroluminescence, showing that chiral clustering by itself is not a sufficient explanation. By injecting spin polarized electrons into the OLED we probe the role of the spin in the production of circular polarized light.

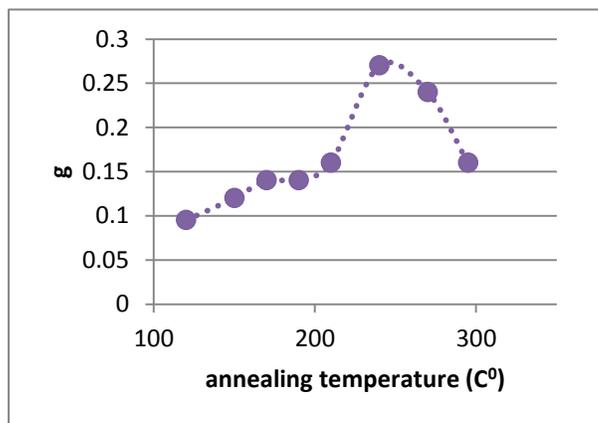


Figure 1. Asymmetry factor of the electroluminescence as a function of the annealing temperature.

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Spin Specific Electron Conduction through Chiral Molecules

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The chiral-induced spin selectivity (CISS) effect entails spin-selective electron transmission through chiral molecules.¹ This is achieved due to the special property of chiral symmetry that couples the electron's spin and its linear momentum so that the molecules transmit one preferred spin over the other.² The spin polarization (SP) is remarkably high and temperature independent. In this study, we focus on two different types of chiral molecules, oligopeptides that possess chiral secondary structure and helicene which does not have stereogenic carbon. Spin selectivity through helicene molecules is demonstrated using magnetic conductive probe atomic force microscopy (mCP-AFM), which revealed that the transmission of one spin is larger by a factor of two as compared to the other spin. Magnetoresistance (MR) of ~2% was measured and it is antisymmetric in respect to the applied magnetic field, unlike a symmetric behavior observed in the conventional magnetoresistance. The present results suggest that the preferred spin is opposite for P and M-enantiomers.³ The spin selectivity through oligopeptides was measured when different force is applied along the molecules. The spin selectivity decreases with increasing applied force, an effect attributed to the increased ratio of radius to pitch of the helix upon compression and increased tilt angles between the molecular axis and the surface normal.⁴

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Biomolecular spin valves based on bacteriorhodopsin

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We report on new type of spin valve which is based on the chirality induces spin selectivity (CISS) effect and show magnetoresistance of $\sim 2\%$ at room temperature. The device is fabricated using self-assembled monolayer of *n*-octylthioglucoside-bacteriorhodopsin (OTG-bR) adsorbed on cysteamine functionalized gold layer and capped with a 2.5 nm thin film of MgO. Thin Ni film on top is used as analyzer. The monolayers of cysteamine and OTG-bR were characterized by polarization modulation-infrared reflection-absorption and atomic force microscopy. These chiral molecules based spin valves show asymmetric magnetoresistance (MR) response when field is applied in the direction of the current since only one kind of spins can be injected through the chiral molecules. A symmetric positive magnetoresistance curve was obtained when field was applied in perpendicular direction to the current. When the analyzer is magnetized in-plane in either direction, the injected spins from chiral layer would scatter more due to all perpendicularly aligned magnetic moments while at zero field, randomly aligned magnetic moments would allow less scattering. We propose that such chiral molecules based spin injector can be applied in molecular spintronics devices.

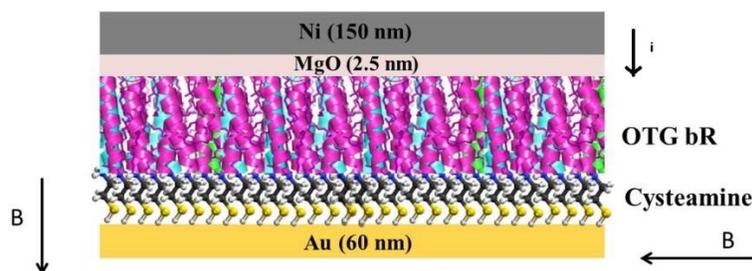


Figure 1. Device structure of the OTG-bR spin valve

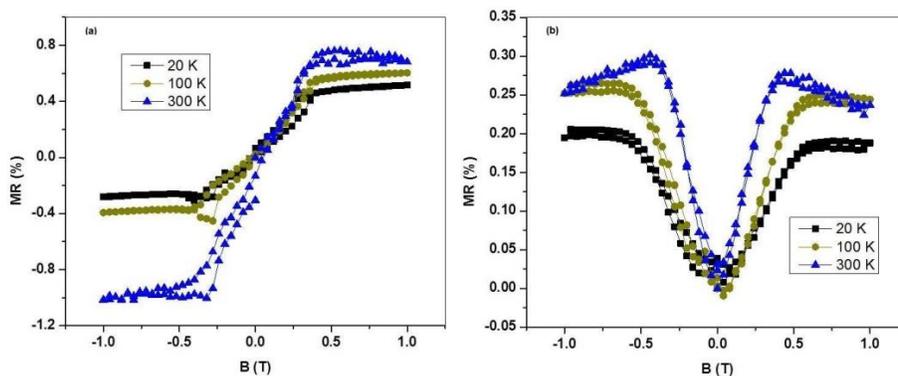


Figure 2. MR curve when magnetic field is applied (a) parallel and (b) perpendicular to current

ams AG. Si and SiN photonics development.

ams is a global leader in the design and manufacture of advanced sensor solutions. Leading manufacturers around the globe rely on ams' sensing know-how for advanced systems design. For ams, "Sensing is Life", and our passion is in creating the sensor solutions that make devices and technology smarter, safer, easier-to-use and more eco-friendly. ams' sensor solutions are at the heart of the products and technologies that define our world today – from smartphones and mobile devices to smart homes and buildings, industrial automation, medical technology, and connected vehicles. Our products drive applications requiring small form factor, low power, highest sensitivity and multi-sensor integration. We offer sensors (including optical sensors), interfaces and related software for consumer, communications, industrial, medical, and automotive markets.

- Focus on optical, environmental, imaging, audio
- High performance sensor solutions, sensor ICs, interfaces & related software
- Small, low power, highest sensitivity, multi-sensor integration
- Best-in-class solutions for leading OEMs
- Full service foundry including packaging and testing options

More than 4,300 employees worldwide, 20 design centers (Europe, Asia, and USA), 35 years of experience.

- Headquarters are located in Premstätten (Styria, Austria).
- Internal wafer manufacturing, Austria
- Internal optical packaging, Singapore
- Manufacturing partnerships for scalability and flexibility
- In-house test, Austria + Philippines

In cooperation with European and Israeli partners, we develop photonics manufacturing processes, active and passive devices, monolithic circuits and hybrid systems for Datacom and sensing solutions.

Our area of interest include silicon nitride based photonics as well as silicon (SOI) for IR operation.

This poster represents the last one: silicon on insulator based manufacturing process (flow and characterization), both passive (grating couplers, waveguides, etc.) and active (modulators) devices.

Mass-Spectrometry Application of Biomolecular Beam in Electrostatic Ion Beam Trap (EIBT)

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ABSTRACT: We have developed a new system that couples an electrospray ion source to an EIBT (Electrostatic Ion Beam Trap). Between the source and EIBT there is a Paul trap in which the ions are accumulated before being extracted and accelerated. The EIBT consist with tow electrostatic mirrors, the first one (entrance) is grounded while the ions are entered. After the ion bunch has entered the EIBT, the ions are trapped by rapidly raising the voltages on the entrance mirror. The ion bunch is oscillating between the mirrors and detected by amplifying the charge induced on a pickup ring in the center of the trap. The ion mass being directly proportional to the square of the oscillation period. Trapping of biomolecules in the in the EIBT is used for calculation of mass spectra and collision cross sections by measuring the different frequencies and lifetimes in the trap. Different setting of the trap that induced selfbunching showed a coalescence of ions of nearby mass.

One-dimensional poly(dimethylsiloxane) dot grating patterns by dip-pen nanolithography

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The invention of dip-pen nanolithography (DPN) in 1999 introduced possibilities for creative scanning probe lithography, forming surface architectures through delivering materials directly with an inked scanning probe [2, 3].

Dip-pen nanolithography (DPN) is a low-cost bottom-top versatile method for directly patterning materials on surfaces with sub-50 nm resolution, it involves the use of a cantilever tip to transfer a selected ink onto various surfaces to create dot and line array patterns, which are then bonded irreversibly to the substrate [1-3].

There are many parameters to consider when attempting to utilize DPN due to the direct transfer of materials to the patterning surface and the chemical interaction between them. DPN tip deposition of liquid inks is not well understood for lack of thorough study of the various parameters which need to be controlled in order to achieve uniform patterning [4].

This work focuses on printing complex patterns of 30 dots [5x6] and 200 μ m or longer lines over a SiO₂ substrate. We have prepared seven different types of Sylgard 184 PDMS based inks diluted with hexane to give varying percentage mixtures (wt%/wt%) and different viscosities. The patterning procedures were performed at a temperature of 23°C, and we examined the effect of the different parameters over the patterning. In addition to the different hexane percentage mixtures, we also observed the effect of humidity and dwell time of the tip on the surface. Overall, we tested three humidity conditions at seven different dwell times of the tip on the surface, with seven different hexane percentages mixtures.

The viscosity and surface tension of each mixture is presented in Table 1. The effect of the humidity conditions was significant mainly at high tip dwell times. We have created a databank which allows the selection of operating conditions and ink types for obtaining the desirable dot diameter and height.

Table 1. The measured viscosity and surface tension of the hexane dilutions

Hexane percentage [wt%]	10	20	30	40	50	60	70
Viscosity [cP]	1343	265.3	117.8	84.43	31.82	18.92	6.224
Surface tension [mN/m]	22.06	21.30	20.75	20.48	20.22	19.89	19.81

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Ground-state Charge Transfer for NIR Absorption with Donor/Acceptor Molecules: Interactions Mediated via Energetics and Orbital Symmetries

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In this work we present a comprehensive experimental study on charge-transfer complex (CPX) formed through orbital hybridization between organic conjugated molecules [1]. Thin films of CPX are prepared by thermal co-evaporation, and are characterized by means of UV/VIS/NIR absorption spectroscopy, ultraviolet photoelectron spectroscopy (UPS), and polarization-modulated IR absorption spectroscopy (PMIRAS). This enables us to explore how orbital symmetry, energy level alignment and steric hindrance impact on orbital hybridization as a green scheme for producing near-infrared active materials [2]. In order to identify the product as CPX rather than physical mixture or charge-transfer salts (integer charge transfer), the following criteria have been examined: ①optical absorption features distinct from those of parental molecules, ②remarkable down-shift in ionization potential (IP) level in films of CPX from that of pristine films of donor molecule, and ③discernable shift of IR absorption of characteristic vibrational modes indicative of partial charge transfer. As a proof-of-principle study, three principles can be drawn out from our experimental results for determining the possibility of orbital hybridization between two candidate molecules, namely, good alignment in IP/EA, absence of steric hindrance, and proper fitting in orbital symmetry.

Keywords: charge transfer, orbital hybridization, NIR, complex, photoelectron spectroscopy

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