

# THE WORKSHOPS

**DIPC facilitates the exchange of information and establishment of new creative research collaborations between attending scientists.**

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## COMELCAN MEETING AND WORKSHOP ON TRANSPORT IN NANOTUBES

JUNE 3-7, 2002

Program Committee

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**The aim of this workshop** is to review the recent advances in the physics of carbon nanotubes, addressing the applications in electron-mechanical devices and nanoelectronics. We address new features and techniques related to the electronic transport through these one-dimensional structures: superconductivity, electron-correlations, quantum coherence, ballistic and coulomb blockade effects, etc. The workshop is complemented with an internal meeting of the COMELCAN research training network as well as a young researchers meeting.

### CONTRIBUTIONS

<i>V. Krstic</i>	<b>Ballistic and electron-correlated transport and other electrical transport phenomena in carbon nanotubes</b>
<i>S. Guéron</i>	<b>Superconductivity in carbon nanotubes</b>
<i>T. Nussbaumer</i>	<b>Superconductor-(NT) Quantum Dot-Superconductor or SNS junctions</b>
<i>M. Grioni</i>	<b>Fermi liquid versus Luttinger liquid in 1D systems: what do we learn from photoemission?</b>
<i>S. Roche</i>	<b>Quantum transport in carbon nanotube based systems</b>
<i>O. Chauvet</i>	<b>Transport properties on SWNT/PMMA</b>
<i>S. Purcell</i>	<b>Current-induced heating of carbon nanotubes during field emission: experiment and modelisation</b>

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## TOWARDS ATOMIC SCALE- AND TIME-RESOLUTION AT INTERFACES

JULY 1-5, 2002

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**The aim of this workshop** is to bring together researchers with backgrounds in theory and experiments in order to assess the present state of our understanding of ultrafast phenomena and atomic control at interfaces in condensed matter, surface science, chemistry, and biology. The idea is to contrast both theoretical and experimental studies to gain insight and establish new links and future collaborations.

## CONTRIBUTIONS

### July 1

- K. Kern*                    **Scanning tunneling microscopy as local probe of electron density and dynamics**
- R. Berndt*                **Probing Electron Dynamics with STM**
- K.-H. Rieder*            **The scanning tunneling microscope as operative tool: Physics and chemistry with single atoms and molecules"**
- Z.W. Gortel*             **The core level clock in free molecules and in adsorbates**
- W. Wurth*                **Ultrafast charge transfer processes at adsorbates investigated using the core level clock**
- D. Menzel*              **Selective bond breaking in adsorbates by core excitations**
- W. Zinth*                **Femtosecond Processes in Primary Photosynthesis: Reactions Optimized for Highest Efficiency**

### July 2

- K. Morgenstern*        **Electron-induced manipulation of water on surfaces: From hexamer formation to dissociation**
- K. Reuter*                **Surface knowledge from ultra-high vacuum to technically-relevant conditions: the example of catalytic CO oxidation**
- A. González Ureña*    **Laser induced charge - transfer processes at adsorbate/metal interfaces**
- M. Wolf*                 **Femtochemistry and ultrafast electron dynamics at adsorbate/metal interfaces**
- M. Bonn*                **Surface dynamics studied with femtosecond vibrational spectroscopy**
- K. Al-Shamery*         **Photoinduced processes at nanoparticulate systems**

### July 3

- G. Dujardin*            **Atomic-scale control of electronic and dynamical processes on semiconductor and insulator surfaces**
- F. Flores*                **Inelastic mean free path for electrons : Ballistic Electron Emission Microscopy**
- W.-D. Schneider*     **Scanning tunneling spectroscopy and microscopy of ultrathin dielectric films**
- U. Höfer*                **Five-wave mixing investigation of electron dynamics at silicon surfaces**
- W. Pfeiffer*             **Ultrafast transport phenomena in metal-insulator-metal contacts**
- H. Petek*                **Ultrafast relaxation of electrons in metals in space, time, frequency domains**
- T. Heinz*                **Combining femtosecond lasers with Scanning Tunneling Microscopy**
- A. Castro*                **Optical Properties of nanostructures: a first-principle approach**

*cont'd*

**July 4**

<i>M. Weinel (Th. Fauster)</i>	<b>Femtosecond dynamics of electrons at surfaces</b>
<i>J.-P. Gauyacq</i>	<b>Effects of adsorbates on image states at metal surfaces</b>
<i>H. Dürr</i>	<b>Probing nanomagnetism on the femtosecond time scale</b>
<i>S. Hufner</i>	<b>Surface state width on noble metal (111) surfaces</b>
<i>M. Persson</i>	<b>Theory of single molecule vibrational spectroscopy and microscopy</b>
<i>T. Frauenheim</i>	<b>Towards theoretical understanding of nanoscale materials functioning and biomolecular processing</b>
<i>E. Chulkov</i>	<b>Momentum Resolved Electron and Phonon Contribution to the Quasiparticle Decay at Metal Surfaces</b>
<i>A. Eiguren</i>	<b>Electron phonon contribution to the lifetime of surface states</b>

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# REUNIÓN NACIONAL DE USUARIOS DE TÉCNICAS DE NEUTRONES

OCTOBER 3-4, 2002

Organizers

*Donostia International Physics Center*

*Sociedad Española de Técnicas Neutrónicas*

*“Unidad Física de Materiales”, Consejo Superior de Investigaciones Científicas*

*Departamento de Física de Materiales (UPV/EHU)*

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**The main goal was the interchange of ideas**, results and expertise among the Spanish neutron scattering users. On the other hand, with this conference – that is intended to be held each year or each two years – we tried to start a series of regular meetings within the Spanish neutron users community. The essence of this kind of conferences is the same as that of other similar meetings that take place periodically in other European countries, organized by the corresponding national associations included in the ENSA (“European Neutron Scattering Association”).

## CONTRIBUTIONS

*J. Luzón*

**Study of the spin density distribution in the molecular magnet O<sub>2</sub>N<sub>2</sub>C<sub>6</sub>F<sub>4</sub>CN<sub>2</sub>SSN by means of polarized neutron diffraction**

*J.M. de Teresa*

**Magnetic clusters in manganites probed with small-angle neutron diffraction**

*A. Señas*

**Pressure effects on TbM<sub>1-x</sub>Cu<sub>x</sub> (M=Pt and Ni) compounds**

*A. Arbe*

**Crossover from Gaussian to Non-Gaussian Behavior in the  $\alpha$ -Relaxation of Polyisoprene**

*C. Cabrillo*

**Microscopic collective excitations in quantum and metallic liquids**



*A. Moreno*

**Methyl group dynamics in the disorder: from rotational tunneling to classical jump**

*G. Cuello*

**Neutron diffraction in liquid and amorphous systems**

*P. Monceau*

**Scientific activities at the Laboratoire Leon Brillouin (LLB) (Saclay, France)**

*Ch. Vettier*

**Fluctuations in Solids : neutrons provide a global view**

*R. Cywinski*

**Muon Beam Research in Condensed Matter Science: Achievements and Prospects**

*C. Frontera*

**Bismut effect on Manganites: a new mechanism for the charge order**

*D. Richter*

**Neutrons in Soft-Condensed Matter Science**

*M.A. González*

**Quasielastic neutron scattering in liquids with hydrogen bonds**

*P. Gorria*

**Study of crystallization kinetics and metastable phase segregation with neutron thermo-diffraction**

*M.A. Castro*

**Alkanes adsorption on graphite surface**

*F. Mezei*

**The ESS Revolution in Neutron Scattering Research Opportunities**

*J. Hernandez*

**Incommensurate Magnetic Structures in R<sub>2</sub>BaCoO<sub>5</sub> Oxides (R=Rare Earth)**

*K. Clausen*

**ESS - the European project to maintain World leadership**

*S. García*

**Hydrogen bonds formation and structural stabilization in laminar and tridimensional phosphates**

*J.J. Blanco*

**Magnetic structure of the phases Sr<sub>2</sub>FeRe<sub>1-x</sub>B<sub>x</sub>O<sub>6</sub> (B= Nb, Ta; x=0,0.1)**

*J.A. Alonso*

**Charge desproportion in the perovskites Rn<sub>1</sub>O<sub>3</sub>**

*cont'd*



*The participants on the grounds of Miramar Palace in San Sebastian*

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MARCH 5-7, 2003

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**Computers and computational methods** have come to play an increasingly important role in natural sciences. In the area of biochemistry, theoretical modeling is for example used to understand the details governing why certain compounds or chemicals are toxic and others are not, how DNA is effected by UV-radiation, or how to design new and more efficient drugs.

During March 5 - 7, the Donostia International Physics Center (DIPC), along with the theoretical chemistry groups of The University of Uppsala and of the UPV/EHU, which are very active in these areas, organized a symposium on theoretical biochemistry/biophysics. The symposium brought together some 50 participants from Europe and North America, including many leading researchers in the field.

Among the many topics covered at the symposium were recent developments of the theoretical toolbox used by the researchers, as well as applications thereof to develop new antitumor drugs, to explain the toxicity of aluminium, or the intriguing fact that lobsters turn red upon cooking.

#### **C O N T R I B U T I O N S**

*R. J. Boyd*

**Towards the development of theoretical models for biological catalysis**

*A. Largo*

**Synthetic routes for interstellar organic and prebiotic molecules**

*J. M. Mercero*

**Aluminum interactions with aminoacid side chains in a protein model environment**

*B. Durbeej*

**Some applications of time-dependent density functional methods to biochemical systems**

*J. Villa*

**Ion channels: through the hole and over the mountain**

*A. González-Lafont*

**On the location of stationary points in enzymatic catalysis: mandelate racemase as an example**

*J. I. Mujika*

**Theoretical study of the cleavage of the peptidic bond**

*R. Stole*

**Ligand binding and conformational changes in DNA gyrase B**

*V. Moliner*

**Theoretical insights in enzyme catalysis**

*N. Russo*

**A DFT investigation of some biomolecular systems**

*U. Ugalde*

**Microbial autoinducers: molecular structure and biological function**

*E. San Sebastian*

**Molecular modelization of antimetastatic drugs and drug targets**

*A. Zubia*

**Antimetastatic drugs: an example of synthesis based on theoretical design**

*X. Lopez*

**QM and QM/MM studies on phosphate diester hydrolysis reactions**

*F. Himo*

**DFT studies of radical enzymes**

*A. Rubio*

**Optical properties of biomolecules within TDDFT: excited state electron ion dynamics**

*M. Duran*

**A new vision of aromaticity through the electron-pair density**

*J. Llano*

**Thermochemistry of electron, proton, and proton-coupled electron transfer reactions in solution**

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**Computational methods for RNA catalysis**

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# PHYSICS MEETS BIOLOGY: SCATTERING AND COMPUTER SIMULATIONS

JUNE 25-28, 2003

Chairmen

*Prof. J. Colmenero* (Universidad del País Vasco/Euskal Herriko Unibertsitatea, Spain)

*Prof. D. Richter* (IFF Jülich, Germany)

**The idea is to put together** a reduced number of experts coming from different but related areas - scattering and computer simulation - in order to explore new routes, ideas and synergies for the future of this field.

## CONTRIBUTIONS

*D. Richter* **Neutron scattering in soft condensed matter**

*J. Colmenero* **Doing MD simulation in polymers as a neutron scattering practitioner**

### SELF ASSEMBLY

*A.R. Khokhlov* **Biomimetic sequence design and evolution of sequences in copolymers**

*A. Semenov* **Hierarchical structure, fibrils and globules in heteropolymer systems**

### PROTEIN DYNAMICS

*F. Parak* **The dynamics of proteins with characteristic times from femtoseconds to microseconds**

### PROTEIN DYNAMICS - NEUTRON SCATTERING AND MODELLING

*J. Smith* **Protein dynamics and hydration: Scattering meets computer simulation**

*M.C. Belissent-Funel* **Internal motions in proteins: a combined neutron scattering molecular modelling approach**

### THE INFLUENCE OF SOLVENTS

*D. Tobias* **Hydration effects**

*A. Sokolov* **Influence of solvents on the dynamics of proteins and DNA**

### PROTEIN FOLDING

*T. McLeish* **Protein folding down to (hyper-)gutter?**

*A. Grosberg* **Title to be announced**

### MEMBRANES

*G. Gompper* **Budding of crystalline domains in fluid membranes**

*D. Roux* **DNA in multilamellar vesicles – a new vector for drug delivery**

## MEMBRANES AND MOLECULAR MACHINES

*E. Goñi*                    **Cell membranes: a few questions for physicists**

*P. Timmins*             **The role of troponin in the regulation of vertebrate muscles**

*Round table discussion*

**Future perspectives of a joined neutron scattering and simulation approach**

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## OPTICAL PROPERTIES OF COMPLEX MATERIALS OVER DIFFERENT LENGTH SCALES

JULY 7-11, 2003

Co-chairmen

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*Prof. F. Meseguer* (Unidad Asociada CSIC-UPV, Valencia, Spain)

*Prof. A. Modinos* (National Technical University of Athens, Greece)

*Prof. J. Pendry* (Imperial College, London, UK)

**The aim of this workshop** is to bring together researchers with backgrounds in theory and experiments in order to assess the present state of our understanding of small particles as building blocks of meta-materials with engineered optical properties. This will cover the interaction of light with both photonic crystals and non-periodic structures at different wavelength scales ranging from the far infrared to the visible, as well as the theoretical and experimental techniques that are needed to investigate them. The main purpose is to combine knowledge about small particle characterization and complex systems of particles to gain insight and establish new links and future collaborations.

This workshop is of special interest to researchers conducting theoretical or experimental studies on:

Effective media and meta-materials

Optics from the nanometer to the millimeter scale

Collective excitations and plasmons

Photonic crystals

Electron diffraction: bridging the gap between electron and radiation waves

Electron microscopy

## CONTRIBUTIONS

<i>T. Ebbesen</i>	<b>Diffraction control and enhanced transmission through sub-wavelength apertures in metal films</b>
<i>L. Martín Moreno</i>	<b>Extraordinary optical properties of nanostructured metals</b>
<i>J. Prikkulis</i>	<b>Light scattering by small holes in thin metal films</b>
<i>M. Sorolla</i>	<b>Electromagnetic band gaps in planar microwave technology</b>
<i>N.I. Zheludev</i>	<b>Fundamental symmetries of light's interaction with planar chiral nanostructures</b>
<i>M. Nieto-Vesperinas</i>	<b>Electromagnetic forces in the near field</b>
<i>T. Heinz</i>	<b>Surface nonlinear optics of nanostructures</b>
<i>E. Ozbay</i>	<b>Physics and applications of 2D and 3D photonic crystals</b>
<i>S. Tretyakov</i>	<b>Physical means to store and amplify evanescent modes</b>
<i>J. B. Pendry</i>	<b>Designing lenses for the near field</b>
<i>R. Marqués</i>	<b>Amplification of evanescent waves and subwavelength focusing in feasible simple physical systems</b>
<i>V. M. Shalaev</i>	<b>Plasmonic nanoantennas for guiding light and sensing molecules</b>
<i>S. Coyle</i>	<b>Chameleon metals-metallic meshes from self-assembled colloids</b>
<i>H. Benisty</i>	<b>Planar photonic crystal: the example of InP-based photonics and the relevant length scales in actual applications</b>
<i>A. Modinos</i>	<b>Photonic band gaps and disorder effects</b>
<i>B. Barnes</i>	<b>Surface plasmon length scales</b>
<i>F. Meseguer</i>	<b>New architectures in opal structures</b>
<i>N. Zabala</i>	<b>Electron energy loss analysis of nanoporous alumina films</b>
<i>N. Yamamoto</i>	<b>Light emission from nano-structures induced by high-energy electron beams</b>
<i>A. Howie</i>	<b>Where is spatially resolved spectroscopy going?</b>
<i>C. Genet</i>	<b>The Casimir force: theory-experiment comparison</b>
<i>A. Dereux</i>	<b>Oxides and metal nanostructures for controlling optical processes at the subwavelength scale</b>
<i>C. N. Afonso</i>	<b>Optical properties of nanostructured metal nanocomposites</b>
<i>M. Käll</i>	<b>Optical properties and applications of gold and silver nanoparticles</b>
<i>J. Aizpurua</i>	<b>Simulating nanoscale optical microscopy and spectroscopy</b>
<i>L. Blanco</i>	<b>Spontaneous emission in the presence of nanostructured materials</b>
<i>D. Wiersma</i>	<b>Complex dielectric systems with external control: from photonic crystal switching to tunable random Laser action</b>
<i>A. Postigo</i>	<b>Photonics crystals in active media: design and fabrication at the IMM</b>
<i>L. Guidoni</i>	<b>Femtosecond dynamics of light transmission through sub-wavelength hole arrays in metallic films</b>

*cont'd*

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# DONOSTIA ENCOUNTERS ON PARTICLE-SOLID INTERACTIONS

## MODIFICATIONS FOLLOWING DIFFERENT INTERACTION PROCESSES AT SURFACES

SEPTEMBER 8-13, 2003

Chairman

*Prof. A. Howie* (University of Cambridge, UK)

Organizers

*Prof. P. M. Echenique* (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

*Prof. A. Arnau* (Universidad del País Vasco / Euskal Herriko Unibertsitatea, Spain)

**The 5th Donostia Encounters** on Particle-Solid Interactions was centered around the topic "Modifications following different interaction processes at surfaces". It was sponsored by the Donostia International Physics Center (DIPC). The chairman of the Conference, Prof. Archie Howie selected the following topics: photon and electron beam damage, charging effects in electron beam irradiation, environmental scanning electron microscopy, ion beam lithography and dry etching, computer simulation of condensed matter processes, ion and molecule scattering at surfaces and ion beam analysis.

### C O N T R I B U T I O N S

#### MANIPULATION IN THE ATOMIC SCALE

*N. Tolk*

**Desorption and damage studies at semiconductor surfaces and interfaces using intense, tunable, ultrafast lasers**

*J.I. Pascual*

**Mode-selective manipulation of the cleavage of a single molecular bond**

#### PHOTOCHEMISTRY AND LOW ENERGY ELECTRONS

*D. Menzel*

**Photochemistry in adsorbates: Coupling-induced modifications, quenching, and selectivity**

*P. Rowntree*

**Interaction of low energy electrons with soft molecular systems**

#### ION BEAM ANALYSIS

*P. Puspa*

**Ion scattering as a tool for material science**

*F. Paszti*

**Interaction of MeV ions with porous materials: morphological changes and their investigation by ion beam analysis**



#### IONS AND ELECTRONS WITH INSULATORS

*J. Cazaux*

**Electron irradiated insulators: mechanisms of charging and correlation with some chemical modifications**

*B. Thiel*

**Control of secondary electron emission from insulating surfaces by soft-landing ions in the low vacuum SEM**

#### SMALL STRUCTURES

*P. Kruit*

**Electron-beam-induced deposition of sub-10 nanometer structures**

*J.R. Sabin*

**Ion Induced Molecular Fragmentation**

#### ENERGY LOSS AND ELECTRON EMISSION

*V.A. Khodyrev*

**The current density approach in treatment of energy loss**

*M.S. Gravielle*

**Differential electron emission spectra produced by grazing ion-surface collisions**

#### ION-SURFACE INTERACTIONS

*P. Bauer*

**Electronic interactions of slow He ions at a metal surface**

*D. Boerma*

**Surface and thin layer physics at the CNAM of the UAM**

#### TECHNOLOGICAL APPLICATIONS

*J. Colligon*

**Modification of surface hardness using ion-assisted deposition**

*W.H. Bruenge*

**Ion projection direct structuring of surfaces: technology and applications**

#### MOLECULES AT SURFACES

*D. Farias*

**Looking at the hydrogen dissociation process via diffraction experiments**

*F. Busnengo*

**Low energy H<sub>2</sub> scattering from metal surfaces: reactivity and dissociation mechanisms**

#### ELECTRONS AND PHOTONS IN CRYSTALS

*N. Vast*

**Anisotropy of the microscopic fluctuations of the polarization, confinement effects, and the dielectric function of crystals**

*E.J. G. de Abajo*

**The Cherenkov effect in photonic crystals**

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*Professors Jacques Cazaux, Peter Kruit and Wilhelm Bruenger*

SEPTEMBER 21-24, 2003

Chairmen

*Prof. R.W. Godby* (York University, UK)

*Prof. A. Rubio* (Universidad del País Vasco, Euskal Herriko Unibertsitatea, Spain)

Organizers

*Dr. P. García-González* (Universidad Autónoma de Madrid, Spain)

*Prof. A. Rubio* (Universidad del País Vasco, Euskal Herriko Unibertsitatea, Spain)

**The aim of this workshop** is to assess the present status of theoretical approaches to the study of spectroscopic properties of real materials, and explore their capability for applications in further systems with technological and biological interest. Due to the different methods used to tackle this problem (Many-Body Theory, Density Functional Theory, Configuration Interaction, semi-empirical approaches), this workshop is intended as a way to promote links among scientists coming from different communities working or interested in electron excited states.

## CONTRIBUTIONS

### THEORETICAL FOUNDATIONS I

*E.K.Gross*

**ELFs and Ghosts in Density Functional Theory**

*Y.M. Niquet*

**High-accuracy XC potentials from the linear-response Sham-Schluter equation: Asymptotic behavior and properties**

### THEORETICAL FOUNDATIONS II

*F. Sottile*

**Parameter-free calculation of response functions in time-dependent density-functional theory**

*A. Marini*

**Bound excitons in time-dependent density-functional-theory: optical and energy-loss spectra**

*S. Biermann*

**Electronic structure of strongly correlated materials-a view from dynamical mean field theory**

### BIOLOGICAL AND ORGANIC SYSTEMS I

*P. Carloni and M. Rohlfing*

**Dynamics of electronically excited molecules**

#### COMPLEX SYSTEMS I

*G. Onida*

**Calculating optical spectra of surfaces and other non infinite systems using plane waves in DFT-LDA and Beyond: bottlenecks and progresses**

*O. Gunnarsson*

**Calculation of dynamical correlation functions: Application to resistivity saturation**

#### COMPLEX SYSTEMS II

*C. Hogan*

**Electron energy loss spectroscopy at As-rich GaAs(001) surfaces**

*M. Friak*

**Ab Initio investigation of the Halfmetal-Metal transition in magnetite**

*K. Tsemekhman*

**Self-Consistent Self-Interaction corrected DFT: The Method and applications to extend and confined systems**

*K. Tatarczyk*

**Surface plasmons in surface alloys**

#### BIOLOGICAL AND ORGANIC SYSTEMS II

*F.J. Himpsel*

**Electronic excitations at the interface between soft and hard matter**

*G. Schmidt*

**Ground-and excited-state properties of small molecular systems: Pyrimidine and purine bases in the gas phase and adsorbed on silicon**

#### BIOLOGICAL AND ORGANIC SYSTEMS IV

*A. Seitsonen*

**TDDFT in molecules and extended systems**

*A. Castro*

#### BIOLOGICAL AND ORGANIC SYSTEMS V

*M. Sulpizi*

**A Hybrid time-dependent density functional/molecular mechanics investigation of aminocoumarins in solution**

*E. Molinari*

**Optics and transport of (bio) molecular systems: solid state effects and P-P interactions**

*A. Calzolari*

**Electron channels in biomolecular nanowires**

*G. Stefanucci*

**Different ways of treating the bias and the inclusion of many-body interactions in the description of quantum conductance**

#### ELECTRON TRANSPORT

*J. G. Herrero*

**Measuring the electrical transport properties of individual molecules: carbon nanotubes and DNA**

*P. Bokes*

**Coherent steady current-carrying states from the maximum entropy principle and the Kubo Formula**

*A. Wacker*

**Nonequilibrium quantum transport in quantum cascade lasers**

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