



FOUNDATION AND CENTRE FOR SCIENTIFIC CULTURE ETTORE MAJORANA
INTERNATIONAL SCHOOL OF SOLID STATE PHYSICS

VIBRATIONS AT SURFACES 12

Erice, Sicily, 20-26 July 2007



San Domenico, Dirac Auditorium

Chair: Giorgio Benedek (Università di Milano-Bicocca, Italy)
Scientific Secretary: Luca Vattuone (Università di Genova, Italy)

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SCHEDULE

	July 21, Sa	July 22, Su	July 23, Mo	July 24, Tu	July 25, We
9.00-10.20	<i>Welcome</i> Ibach Theis	Tautz Pratt	Kroger Chulkov	Dujardin Sloan	Allison Farias
10.20-11.00	Sachert Schennach	Delebecque Pradier	Gaal-Nagy Chis	Pettinger Ueba	Gumhalter Manson
	<i>Break</i>	<i>Break</i>	<i>Break</i>	<i>Break</i>	<i>Break</i>
11.20-12.00	Bartels	Witte	Bird	Tolk	Murphy
12.00-12.40	Lorente	Savio	Hellsing	Kudelski Miyauchi	Tysoe
12.40-13.00	Kim	Okada	Muino	Bourguignon	Arafune
	<i>Lunch</i> <i>Break</i>	<i>Lunch</i> <i>break</i>	<i>Lunch</i>	<i>Lunch</i> <i>break</i>	<i>Lunch</i> <i>Break</i>
15.40-16.20	Tadjeddine	Reis	<i>Excursion to the archeological site of Selinunte</i>	Hong	Franchini
16.20-17.00	Busson Han	Wolf Li-Wei		Alc.-Ortigoza Beyvers	Persson Darling
	<i>Break</i>	<i>Break</i>		<i>Break</i>	<i>Break</i>
17.20-18.00	Bonn	<i>Poster presentations</i>		<i>Swimming and dinner at Marinella</i>	<i>Poster presentations</i>
18.00-18.40	Bernasconi		<i>Poster Session I</i>		
18.40-19.40	Humbert Keszthelyi Onda				
	<i>Dinner</i>	<i>Dinner</i>		<i>Dinner</i>	<i>Banquet</i>



Friday, July 20th, 2007

21.00-24.00 After-dinner GET-TOGETHER at the Marsala Room in San Rocco

Saturday, July 21st, 2007

9.00-9.15 *Welcome*

Opening Session – Chair: G. Benedek

9.15-10.00 **H. Ibach** (Research Center Jülich, Germany)
Why and to what end are we pursuing surface vibration spectroscopy **Sa-I1**

Session: Molecular processes and devices I - Chair: M. Rocca

10.00-10.20 **W. Theis** (Freie Universität Berlin, Germany)
Surface phase transition in H/W(110) induced by tuning the Fermi surface nesting vector by Hydrogen loading Sa-O1

10.20-10.40 **S. Sachert** (Martin-Luther-Universität Halle-Wittenberg, Halle, Germany)
Vibrational and structural properties of manganese oxide ultrathin films on Pt(111): An HREELS and STM study Sa-O2

10.40-11.00 **R. Schennach** (Graz University of Technology, Graz, Austria)
Adsorption and Reaction of CO on Rh(111) and Rh(553) Sa-O3

11.00-11.20 Coffee break

Session: Single-molecule Spectroscopy I - Chair: H. Ueba

11:20-12.00 **L. Bartels** (University of California at Riverside, USA)
Dynamics of Individual Molecules at Cu(111) **Sa-I2**

12.00-12.40 **N. Lorente** (CSIC, Barcelona, Spain & Univ. Paul Sabatier, Toulouse, F)
Vibrational excitation by tunnelling electrons: reactivity and spectroscopy **Sa-I3**

12.40-13.00 **Y. Kim** (Surface Chemistry Laboratory, RIKEN, Japan)
Action spectroscopy for vibrationally-induced motion of a single molecule with an STM Sa-O4

13.00-15.40 Lunch break

Session: Non-linear Spectroscopy I - Chair: D. Reis

- 15.40-16.20** **A. Tadjeddine** (UDIL - CNRS, Centre Universitaire Paris-Sud, France)
Sum frequency generation as a vibrational probe of the interface and thin films **Sa-I4**
- 16.20-16.40 **B. Busson** (LCP/CLIO – CNRS, Université Paris-Sud, France)
Doubly-Resonant Sum-Frequency Generation Properties of Chiral Thin Films Sa-O5
- 16.40-17.00 **X. Han** (University Duisburg-Essen, Germany)
Vibrational relaxation of adsorbates at semiconductor surfaces: H on Ge(100) Sa-O6
- 17.00-17.20 Coffee break

Session: Non-linear Spectroscopy II- Chair: T. Orlando

- 17.50-18.00** **M. Bonn** (FOM-AMOLF, Amsterdam, The Netherlands)
Two-Dimensional Surface Vibrational Spectroscopy **Sa-I5**
- 18.00-18.40** **M. Bernasconi** (Università di Milano-Bicocca, Italy)
Simulation of diffusion and chemical reactions at the surface of silicon by ab-initio metadynamics **Sa-I6**
- 18.40-19.00 **C. Humbert** (Université de Paris-Sud, France)
Two-colour sum-frequency generation spectroscopy with the CLIO free electron laser Sa-O7
- 19.00-19.20 **T. Keszthelyi** (Chemical Research Centre, Budapest, Hungary)
Investigations of interfacial phenomena of biological relevance by sum-frequency vibrational spectroscopy Sa-O8
- 19.20-19.40 **K. Onda** (Tokyo Institute of Technology, Japan)
Nature of Photo-Induced Phase and Coherent Phonon in Organic Conductor (EDO-TTF)₂PF₆ Sa-O9
- 20.00 - Dinner

Sunday, July 22nd, 2007

Session: Molecular Processes and Devices II - Chair: H. Ibach

- 9.00-9.40** **F. S. Tautz** (Jacobs University Bremen, Germany)
Bonding, structure and function of highly ordered molecular adsorbate layers on metal surfaces **Su-I1**
- 9.40-10.20** **S. Pratt** (Department of Chemistry, University of Cambridge, UK)
Structure, symmetry, chirality and enantiospecificity of single-crystal metal surfaces **Su-I2**
- 10.20-10.40 C.M. Pradier (Université Pierre et Marie Curie, France)
PM-RAIRS for Structural and Quantitative Chemical Characterisation of Biological Interfaces Su-O1
- 10.40-11.00 A. Delebecque (Université Pierre et Marie Curie, Paris 6, France)
On the reactivity of NO/N₂ mixture with aluminium surfaces: a combined PM-IRRAS and QCM investigation Su-O2
- 11.00-11.20 Coffee break

Session: Molecular Processes and Devices III - Chair: D. Bird

- 11.20-12.00** **G. Witte** (Ruhr-University Bochum, Germany)
Organic molecular beam deposition of thin films: the influence of substrate interaction **Su-I3**
- 12.00-12.40** **L. Savio** (CNISM & IMEM-CNR, Università di Genova, Italy)
Oxygen interaction with stepped metal surfaces: Ag vs Cu **Su-I4**
- 12.40-13.0 M. Okada, (Osaka University and PRESTO - JSTA, Japan)
Role of Steps in Oxide Formation on Stepped Cu Surfaces using a Hyperthermal O₂ Molecular Beam Su-O3
- 13.00-15.40 Lunch

Session: Non-linear Spectroscopy III - Chair: A. Tadjeddine

- 15.40-16.20** **D. A. Reis**, FOCUS Center and Department of Physics,
University of Michigan (USA)
Ultrafast vibrational spectroscopy using x rays **Su-I5**
- 16.20-16.40 Martin Wolf, Department of Physics, Freie Universität Berlin (Germany)
*Excitation of coherent phonons at surfaces probed by time-resolved
photoelectron spectroscopy* Su-O4
- 16.40-17.00 Li-Wei Chou, Department of Chemical Engineering,
National Taiwan University of Science and Technology (Taiwan)
*Surface Raman spectroscopy of trans-stilbene on
Ag/Ge(111)-($\sqrt{3}\times\sqrt{3}$)R30°: surface-induced effects* Su-O5
- 17.00-17.20 Coffee break
- 17.20-19.40** **Poster and product presentation – Poster Session I**
- 20.00- 23.00 Dinner



Erice: The Norman Castle

Tuesday, July 24th, 2007

Session: Single-molecule Spectroscopy II - Chair: L. Bartels

- 9.00-9.40** **G. Dujardin** (Université de Paris-Sud, Orsay, F)
Localised electronic spectroscopy inside a single molecule **Tu-I1**
- 9.40-10.20** **P. A. Sloan** (The University of Birmingham, Edgbaston, UK)
*Self-assembled halo-alkanes on a semiconductor surface:
charge corralling and electronic switching* **Tu-I2**
- 10.20-10.40 **B. Pettinger** (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)
Tip-enhanced Raman Spectroscopy: Toward Single-Molecule Detection Tu-O1
- 10.40-11.00 **H. Ueba** (University of Toyama, Toyama, Japan)
Action spectroscopy for single molecule motion Tu-O2
- 11.00-11:20 Coffee break

Session: Non-linear Spectroscopy IV- Chair: M. Bonn

- 11.20-12.00** **N. Tolk** (Vanderbilt University, Nashville TN, USA)
*Ultra-fast Laser Induced Vibrational Dynamics at Surfaces Leading
to Bond Scission and Traveling Phonon Wave Induced Oscillations* **Tu-I3**
- 12.00-12.20 **A. Kudelski** (Warsaw University, Warsaw, Poland)
*Local monitoring of surface chemistry with surface-enhanced Raman
spectroscopy* Tu-O3
- 12.20-12.40 **Y. Miyauchi** (JAIST, Ishikawa, Japan)
Electronic and vibrational resonant images of H-Si(111) surfaces Tu-O4
- 12.40-13.00 **B. Bourguignon** (LPM-CNRS, Université de Paris-Sud, France)
*"Full" Modelling of Sum Frequency Generation spectra of CH
modes in Self-Assembled Molecules : implication for the surface
structure of alkyl chains* Tu-O5
- 13.00 15.40 Lunch break



EMCSC: San Rocco

Session: Theory of Surface Dynamical Phenomena I - Chair: G.P. Brivio

- 15.40-16.20** **Sampyo Hong** (University of Central Florida, Orlando, USA)
What can we still learn from surface phonon dispersion curve of chemisorbed systems? **Tu-I4**
- 16.20-16.40 **M. Alcántara Ortigoza**, (Kansas State University, Manhattan, USA)
The dispersion of surface phonons of CO on Cu(100): insights from first-principles calculations **Tu-O6**
- 16.40-17.00 **S. Beyvers** (Institut für Chemie, Universität Potsdam, Germany)
Vibrational IR-excitation in a 3-dimensional, dissipative model of CO/Cu(100) **Tu-O7**
- 17.00-17.20 Coffee break

17.20-19.40 Poster and product presentation - Poster session II

20.00 – 23:00 Dinner

Wednesday, July 25th, 2007

Session: Scattering Spectroscopy I - Chair: E. V. Chulkov

- 9.00-9.40** **W. Allison** (Cavendish Laboratory, University of Cambridge UK)
Dynamics of atoms and molecules at surfaces probed by interferometry with atomic beams **We-I1**
- 9.40-10.20** **D. Farías** (Universidad Autónoma de Madrid, Cantoblanco, Spain)
Probing reaction dynamics at metal surfaces with H₂ diffraction **We-I2**
- 10.20-10.40 **B. Gumhalter** (Institute of Physics, Zagreb, Croatia)
Suppression of inelastic bound-state resonance effects by enlargement of the manifold of quantum paths in atom scattering from surface phonons **We-O1**
- 10.40-11.00 **J. R. Manson** (Clemson University, Clemson SC, USA)
Atomic and Molecular Collisions with Surfaces: Comparisons of Ar and N₂ Scattering from Ru(0001) **We-O2**
- 11.00-11.20 Coffee break

Session: Scattering Spectroscopy II - Chair: W. Allison

- 11.20-12.00** **Murphy B.M.** (Christian-Albrechts-Universität, Kiel, Germany)
IXS: Surface Phonons **We-I3**
- 12.00-12.40** **Wilfred T. Tysoe** (University of Wisconsin, Milwaukee, USA)
*Probing Reaction Pathways on Model Catalyst Surfaces:
Vinyl Acetate Synthesis and Olefin Metathesis* **We-I4**
- 12.40-13.00 **R. Arafune** (PRESTO, JST, Japan)
Inelastic interaction between photoelectrons and surface vibrations We-O3
- 13.00-15.40 Lunch break

Session: Theory of Surface Dynamical Phenomena II- Chair: T. Rahman

- 15.40-16.20** **A. Franchini** (CNISM, Università di Modena e Reggio Emilia, Italy)
Molecular Dynamics Simulations of static friction at the N₂/Pb interface **We-I5**
- 16.20-16.40 **B.N.J. Persson** (IFF, FZ-Julich, Germany)
Heat transfer at Surfaces We-O4
- 16.40-17.00 **G. Darling** (University of Liverpool, United Kingdom)
*H recombination at an ordered SnCu alloy surface:
Reaction dynamics in a bistable system* We-O5
- 17.00-17.20 Coffee break

Session: Theory of Surface Dynamical Phenomena III- Chair: J. R. Manson

- 17.20-18.0** **N. Manini**, (CNR-INFN, Università di Milano, SISSA & CNR-INFN
Democritos National Simulation Center, Trieste, Italy)
*Static friction on the fly: velocity depinning transitions
of lubricants in motion* **We-I6**
- 18.00-18.20 **E. S. Syrkin** (Natl. Academy of Sciences of Ukraine, Kharkov, Ukraine)
*Fano-like Interference Phenomena in Transmission of Elastic Waves
through an Interface between two Solids* We-O6
- 18.20-18.40 **W. Steurer** (Graz University of Technology, Austria)
Observation of the Boson Peak at the Surface of Vitreous Silica We-O7

18.40-19.0 M. Castellà-Ventura (Laboratoire de Dynamique, Interactions et Réactivité, Thiais (France)
Vibrational Analysis of Aza-Aromatic Molecules Adsorption on the Brønsted Acid Sites of Zeolite Surfaces Based on DFT Calculations

We-O8

19.00-19.40 Closing Session

20.00-23.00 Banquet



**The city of Trapani as seen from Erice
and the three Egadi Islands:
Favignana (left), Levanzo (right) and Marettimo (far right)**

Thursday, July 26th, 2007

Departures (pick-up times from your room are listed at the entrance of San Rocco: please check!)

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