



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> <b>Ibach</b> Theis	<b>Tautz</b> <b>Pratt</b>	<b>Kroger</b> <b>Chulkov</b>	<b>Dujardin</b> <b>Sloan</b>	<b>Allison</b> <b>Farias</b>
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	<b>Tolk</b>	<b>Witte</b>	<b>Bird</b>	<b>Bartels</b>	<b>Murphy</b>
12.00-12.40	Kudelski Miyauchi	<b>Savio</b>	<b>Hellsing</b>	<b>Lorente</b>	<b>Tysoe</b>
12.40-13.00	Bourguignon	Okada	Muino	Kim	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	<b>Tadjeddine</b>	<b>Reis</b>	<i>Excursion to the archeological site of Selinunte</i>	<b>Hong</b>	<b>Franchini</b>
16.20-17.00	Busson Han	Wolf Li-Wei		Alc.-Ortigoza Beyvers	Persson Kosevich
	<i>Break</i>	<i>Break</i>		<i>Break</i>	<i>Break</i>
17.20-18.00	<b>Bonn</b>	<i>Poster presentations</i>		<i>Swimming and dinner at Marinella</i>	<i>Poster presentations</i>
18.00-18.40	<b>Bernasconi</b>		Poster session II		Syrkin Steurer Castellà
18.40-19.40	Humbert Keszthelyi Onda	Poster Session I			<i>Closing session</i>
	<i>Dinner</i>	<i>Dinner</i>		<i>Dinner</i>	<i>Banquet</i>



## Friday, July 20<sup>th</sup>, 2007

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

## Saturday, July 21<sup>st</sup>, 2007

**9.00-9.15** *Welcome*

9.00-9.16

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

**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* **Sa-I2**

12.00-12.20 **A. Kudelski** (Warsaw University, Warsaw, Poland)  
*Local monitoring of surface chemistry with surface-enhanced Raman spectroscopy* Sa-O4

12.20-12.40 **Y. Miyauchi** (JAIST, Ishikawa, Japan)  
*Electronic and vibrational resonant images of H-Si(111) surfaces* Sa-O5

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* Sa-O6

13.00-15.40 Lunch break

*Session: Non-linear Spectroscopy II - Chair: N. Tolk*

- 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-I3**
- 16.20-16.40 **B. Busson** (LCP/CLIO – CNRS, Université Paris-Sud, France)  
*Doubly-Resonant Sum-Frequency Generation Properties of Chiral Thin Films* Sa-O7
- 16.40-17.00 **X. Han** (University Duisburg-Essen, Germany)  
*Vibrational relaxation of adsorbates at semiconductor surfaces: H on Ge(100)* Sa-O8
- 17.00-17.20 Coffee break

*Session: Non-linear Spectroscopy III- Chair: T. Orlando*

- 17.50-18.00** **M. Bonn** (FOM-AMOLF, Amsterdam, The Netherlands)  
*Two-Dimensional Surface Vibrational Spectroscopy* **Sa-I4**
- 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-I5**
- 18.40-19.00 **C. Humbert** (Université de Paris-Sud, France)  
*Two-colour sum-frequency generation spectroscopy with the CLIO free electron laser* Sa-O9
- 19.00-19.20 **T. Keszthelyi** (Chemical Research Centre, Budapest, Hungary)  
*Investigations of interfacial phenomena of biological relevance by sum-frequency vibrational spectroscopy* Sa-O10
- 19.20-19.40 **K. Onda** (Tokyo Institute of Technology, Japan)  
*Nature of Photo-Induced Phase and Coherent Phonon in Organic Conduct or (EDO-TTF)<sub>2</sub>PF<sub>6</sub>* Sa-O11
- 20.00 - Dinner

## Sunday, July 22<sup>nd</sup>, 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/N<sub>2</sub> 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 O<sub>2</sub> Molecular Beam* Su-O3
- 13.00-15.40 Lunch



*Session: Non-linear Spectroscopy IV - 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 24<sup>th</sup>, 2007

*Session: Single-molecule Spectroscopy I - Chair: B. N. J. Persson*

- 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: Single-molecule Spectroscopy II - Chair: H. Ueba*

- 11:20-12.00** **L. Bartels** (University of California at Riverside, USA)  
*Dynamics of Individual Molecules at Cu(111)* **Tu-I3**
- 12.00-12.40** **N. Lorente** (CSIC, Barcelona, Spain & Univ. Paul Sabatier, Toulouse, F)  
*Vibrational excitation by tunnelling electrons:  
reactivity and spectroscopy* **Tu-I4**
- 12.40-13.00 **Y. Kim** (Surface Chemistry Laboratory, RIKEN, Japan)  
*Action spectroscopy for vibrationally-induced motion of a single  
molecule with an STM* Tu-O3
- 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-I5**
- 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-O4**
- 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-O5**
- 17.00-17.20 Coffee break
- 17.20-19.40 Poster and product presentation - Poster session II**
- 20.00 – 23:00 Dinner

**Wednesday, July 25<sup>th</sup>, 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 H<sub>2</sub> 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 N<sub>2</sub> 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 (JST, Tohoku University, 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 N<sub>2</sub>/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 Yu. A. Kosevich (Semenov Institute of Chemical Physics, Russian  
Academy of Sciences, Moscow, Russia)  
*Energy Transfer in Coupled Nonlinear Vibration Waveguides:  
Transition from Wandering Breathers to Nonlinear Self-Trapping* **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-INFM, Università di Milano, SISSA & CNR-INFM  
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  
Brönsted 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)**

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**Thursday, July 26<sup>th</sup>, 2007**

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