

# **XXIV Reunión Nacional y VIII Congreso Ibérico de ESPECTROSCOPIA**

**ABSTRACT BOOK**



**XXIV RNE - VIII CIE  
ESPECTROSCOPIA**

Logroño, 9-11 de julio de 2014

## **Martes 8 de julio**

17:00-19:00 Recogida de documentación

19:30 **Vino de bienvenida**

## **Miércoles 9 de julio**

09:00 Sesión de apertura

### **Sesión I, presidida por M<sup>a</sup> Paz Sevilla Sierra**

09:30 Conferencia Plenaria

#### **PL-1. Concepción Domingo**

Raman Spectroscopy, a “broad-spectrum” tool: from rock art to Mars exploration; from graphene-based materials to medical diagnosis or cosmetics industry

10:15 Conferencia Invitada

#### **IL-1. Martín Resano**

Non-invasive methods for clinical elemental analysis. Direct analysis of dried matrix spots for diagnosis and control

10:45 **Café**

### **Sesión II, presidida por María Paula Marques y Belén Maté Naya**

11:15 Conferencia Invitada

#### **IL-2. Helena Vieira Alberto**

Spectroscopy of a muonium atom formed inside a semiconductor

11:45 Comunicaciones Orales: Nanotecnología

O-01. *Diameter selection of carbon nanotubes in arrays of polymer/SWCNT nanowires by template wetting*

M.C. García-Gutiérrez, C. Domingo

O-02. *Synthesis and study of plasmonic properties of gold-silver nanostructures: From a spherical nanoparticles to ultrathin nanowires*

J. Crespo, A. Falqui, J.M. López-de-Luzuriaga, M. Monge, M. E. Olmos, M. Rodríguez-Castillo, M. Sestu, K. Soulantica

O-03. *Gaps induced by molecular linkage of plasmonic nanoparticles in colloidal suspensions for SERS enhanced pesticide sensing*

S. Sánchez-Cortés, J. Kubackova, D. Jancura, J.V. García-Ramos

O-04. *An ICPMS-based analytical platform for the determination of nanoparticles released from nanocomposites*

E. Bolea, I. Abad-Álvaro, J. Jiménez-Lamana, N. Manninen, A. Cavaleiro, S. Carvalho, F. Laborda, J.R. Castillo

O-05. *A novel quantum dot-based phosphorescent immunoassay for PSA detection in human serum: signal amplification strategies based on ICP-MS*

M. García-Cortés, M.T. Fernández-Argüelles, J.M. Costa-Fernández, J. Ruiz Encinar, A. Sanz-Medel

O-06. *Bioconcentration and toxicity studies of titanium dioxide nanoparticles by zebrafish embryos*

R. Muñoz-Olivas, A. López-Serrano, J. Sanz, S. Rainieri, C. Cámera

O-07. *Experimental observation of Fano- and Lorentz-like line shapes in the optical extinction of plasmonic nanorods*

F. López-Tejeira, N. Verellen, R. Paniagua-Domínguez, D. Vercruyse, D. Denkova, L. Lagae, P. Van Dorpe, V.V. Moshchalkov, J.A. Sánchez-Gil

13:30 **Comida**

**Sesión III, presidida por Manuel Hernández Córdoba y María Teresa Tena Vázquez de la Torre**

15:30 Conferencia Plenaria

**PL-2. Demetrios Anglos**

Art and Archaeology through the spectroscopic looking glass

16:15 Comunicaciones Orales: Plasmas

O-08. *Biomedical applications of laser induced breakdown spectroscopy in bacterial identification*

S. Manzoor, S. Moncayo, F. Navarro-Viloslada, J.A. Ayala, R. Izquierdo-Hornillos, F.J. Manuel de Villena, J.O. Cáceres

O-09. *LIBS quantitative analysis of fluorite ores ( $\text{CaF}_2$ ) through the measurement of  $\text{CaF}$  molecular emission bands*

C. Álvarez, J. Pisonero, N. Bordel

O-10. *Different approaches for the generation of chemical maps of complex samples by laser-induced plasma spectroscopy*

M.P. Mateo, G. Nicolás

17:00 Comunicaciones orales: Casas comerciales I

O-11. *MIR-FIR spectroscopy in one step – wide range infrared technology*

C. Villar Pascual, G. Zachmann

O-12. *Spectral interferences removal in multiple isotope selenium and iodine determinations using an ICP-MS triple quadrupole in MS/MS mode*

N. Sugiyama, Y. Shikamori, K. Nakano, S. Kakuta, F. Tobalina

17:30 **Café**

17:30-19:30 **Sesión de carteles 1**

Exhibición Comercial

20:30 **Visita a la calle Laurel (bono-pincho)**

## Jueves 10 de julio

### Sesión IV, presidida por María Cruz Moreno Bondi y José Manuel Costa Fernández

09:00 Conferencia Plenaria

#### PL-3. Luca Prodi

Dye doped silica nanoparticles as luminescent organized systems for nanomedicine

09:45 Conferencia Invitada

#### IL-3. Fernando Rull

Applications of Raman spectroscopy: from the historical heritage to the space exploration

10:15 Comunicaciones Orales: Alimentos y sensores

#### O-13. *β-Cyclodextrin modified CdSe/ZnS quantum dots as a vanillin-sensor*

A. Ríos, G.M. Durán, A.M. Contento

#### O-14. *Furfural selective colorimetric sensors for beer ageing monitoring*

A. Rico-Yuste, E. Benito-Peña, V. González-Vallejo, M.C. Moreno-Bondi

#### O-15. *Determination of technological maturity of grapes and total phenolic compounds of grape skins in red and white cultivars during ripening by near infrared hyperspectral image: A preliminary approach*

J. Nogales-Bueno, J.M. Hernández-Hierro, F.J. Rodríguez-Pulido, F.J. Heredia

11:00 Café

11:30-13:30 Sesión de carteles 2

Exhibición Comercial

13:30 Comida

### Sesión V, presidida por Santiago Sánchez Cortés y Santiago MasPOCH Andrés

15:30 Conferencia Invitada

#### IL-4. Manuel Montejo

Molecular and supramolecular chirality by VCD spectroscopy and quantum chemical calculations

16:00 Comunicaciones Orales: Análisis forense y bioquímico

#### O-16. *Double confirmation of MDMA abuse: saliva analysis*

S. Armenta, S. Garrigues, M. de la Guardia, J. Brassier, M. Alcalá, M. Blanco

#### O-17. *Evaluation of confocal Raman spectroscopy to identify gunshot residue particles*

M. López-López, C. García-Ruiz

#### O-18. *Porous membrane protected molecularly imprinted polymer based microsolid phase extraction for cocaine and metabolites assessment in human plasma by HPLC-MS/MS*

S. García-Carballal, J. Sánchez-González, A.M. Bermejo, M.J. Tabernero, P. Bermejo-Barrera, A. Moreda-Piñeiro

#### O-19. *Determination of lidocaine in urine at low ppm levels using dispersive microextraction and attenuated total reflectance-Fourier transform infrared measurements of dry films*

A. Sánchez-Illana, D. Pérez-Guaita, S. Garrigues, M. de la Guardia

17:00 Café

## **Sesión VI, presidida por José Miguel Vadillo Pérez**

17:30 Comunicaciones orales: Casas comerciales II

O-20. *Supercontinuum fiber lasers: White light with laser brightness. A new tool for advanced spectroscopy*

P. Pérez-Millán, E. Ribes, J.L. Cruz, A. Díez, Y.O. Barmenkov, M.V. Andrés

O-21. *Time-resolved spectroscopy using streak cameras*

J. Sobrino

O-22. *AFM for high resolution and high speed chemical imaging and first fully-integrated Raman Imaging + Scanning Electron microscope (RISE)*

E. Bailo, J. Toporski, U. Schmidt

O-23. *Improving analysis of large isotopes ratios using high sensitivity ICPMS*

P. Cano, M. Hamester, R. Chemnitzer

18:30 **Asambleas de Sociedades**

19:30 Salida de autobuses desde Edificio Quintiliano

20:00 Visita y cena en bodega Campo Viejo

**Viernes 11 de julio**

## **Sesión VII, presidida por Pilar Bermejo Barrera y Luis Batista de Carvalho**

09:30 Conferencia Plenaria

**PL-4. Mario Berberan-Santos**

Thermally activated delayed fluorescence. Fundamentals and applications in optical sensing and in OLED materials.

10:15 Comunicaciones Orales: Análisis ambiental

O-24. *Molecularly imprinted polymer based – solid phase extraction for mercury speciation in seawater by HPLC-ICP-MS*

M.P. Rodríguez-Reino, R. Domínguez-González, P. Bermejo-Barrera, A. Moreda-Piñeiro

O-25. *First insights into mercury speciation in aquatic plants using coupled techniques based on gas chromatography and atomic fluorescence detection*

M. Jiménez-Moreno, M.A. Lominchar, M.J. Sierra, R. Millán, R.C. Rodríguez Martín-Doimeadios

O-26. *FAPA-APGD as ion source for VOCs detection by a novel ion differential mobility analyser*

M. Bouza, J. Orejas, S. López-Vidal, J. Pisonero, N. Bordel, R. Pereiro, A. Sanz-Medel

O-27. *Analytical environmental nanoscience: A new challenge for Analytical Chemistry in the XXI century*

J.R. Castillo, P. Bermejo-Barrera, F. Laborda, E. Bolea, M.S. Jiménez, M.T. Gómez, G. Cepriá, A. Moreda, M.C. Barciela

11:15 **Café**

**Sesión VIII, presidida por Concha Domingo y Carmen Cámará Rica**

11:45 Comunicaciones Orales: Estructura atómica y molecular, materiales avanzados y otros

O-28. *Unveiling the early history of ultrafast laser ablation: Design, construction and evaluation of a femtosecond-resolved phase-change microscope*

I.M. Carrasco-García, M. López-Claros, J.M. Vadillo, J.J. Laserna

O-29. *Copper(II) complexes of cinnamic and caffeic acids: A Raman study*

N.F.L. Machado, M.P.M. Marques

O-30. *Crystal disruption in novel titanias for enhanced photocatalytical applications*

M. Rico-Santacruz, E. Serrano, A. Sepúlveda, E. Lalinde, J. Berenguer, J. García-Martínez

O-31. *Trimeric gold-mercury containing species as fluorescence quenchers*

D. Pascual, J.M. López de Luzuriaga, M. Monge, M.E. Olmos

O-32. *Insights into the coordination chemistry in the system [Zn(I-Lac)(H<sub>2</sub>O)<sub>2</sub>]<sup>+</sup> from DFT, NBO and QTAIM: Structure/vibrational spectra relationship*

M.C. Ramírez Avi, A.A. Márquez García, F. Partal Ureña

O-33. *SCA methodology for the analysis of deposited atmospheric particles on the surface of outdoors exhibited steel sculptures*

J. Aramendia, L. Gómez-Nubla, K. Castro, J.M. Madariaga

O-34. *Raman, SERS and DFT analysis of mauve dye and its components*

M.V. Cañamares, J.R. Lombardi

13:30 **Clausura y entrega de premios**

## Experimental observation of fano- and Lorentz-like line shapes in the optical extinction of plasmonic nanorods

**F. López-Tejeira<sup>1</sup>, N. Verellen<sup>2,3</sup>, R. Paniagua-Domínguez<sup>4</sup>, D. Vercruyse<sup>3,2</sup>, D. Denkova<sup>2</sup>, L. Lagae<sup>3,2</sup>, P. Van Dorpe<sup>3,2</sup>, V. V. Moshchalkov<sup>2</sup>, and J. A. Sánchez-Gil<sup>4</sup>.**

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(2) SINPAC and Dept. of Physics and Astronomy, KU Leuven, Leuven.

(3) IMEC, Leuven, Belgium.

(4) Instituto de Estructura de la Materia, Consejo Superior de Investigaciones Científicas, Madrid, Spain.

Metallic nanorods are widely used as generic plasmonic dipole antennas operating at optical and near-infrared frequencies, forming an analogue to classical half-wave dipole antennas. The fundamental dipole and higher order antenna modes have been extensively studied experimentally using optical spectroscopy and a broad range of mapping techniques. Likewise, theoretical investigations have elucidated the antenna modes' scaling properties, their dependence on the shape, size, and dielectric environment by using a variety of methods. Despite this large interest in nanorods, only very few theoretical reports address the scattering behavior with a focus on the spectral line shape [1-3].

Plasmon resonance, as a wave phenomenon, is expected to present interference characteristics. For localized surface plasmon resonances, interference of spectrally overlapping and coupled modes is well recognized to affect the scattering behavior of the nanostructure under investigation [4, 5]. In particular, the interference of a broad background continuum state with spectrally sharp higher order resonances can lead to a spectral response with asymmetric Fano-like line shapes in a variety of nanoparticle configurations. Only recently, it was indicated that Fano resonances may appear for individual nanorods provided that interacting modes overlap in both spatial and frequency domains [1, 2]. Interestingly, the narrow asymmetrical line shape of a nanorod's Fano interference is, for example, more favorable for label-free biosensing than broader Lorentzian resonances [3].

In our present work [6], we study the spectral line shapes of metallic nanorod antennas in detail, using extinction spectroscopy and finite element simulations. Surface plasmon resonances of odd mode parity present Fano interference in the scattering cross-section resulting in asymmetric spectral lines. Contrarily, modes with even parity appear as symmetric Lorentzian lines. The emergence of either constructive or destructive mode interference is explained with a semi-analytical 1D line current model. This simple model directly explains the mode-parity dependence of the Fano-like interference. Plasmonic nanorods are widely used as half-wave optical dipole antennas. Our findings offer a perspective and theoretical framework for operating these antennas at higher order modes.

### References

- [1] J. M. Reed, H. Wang, W. Hu, S. Zou. Shape of Fano resonance line spectra calculated for silver nanorods. Opt. Lett. 36 (2011) 4386.
- [2] F. López-Tejeira, R. Paniagua-Domínguez, R. Rodríguez-Oliveros, J. A. Sánchez-Gil. Fano-like interference of plasmon resonances at a single rod-shaped nanoantenna. New. J. Phys. 14 (2012) 023035.
- [3] F. López-Tejeira, R. Paniagua-Domínguez, J. A. Sánchez-Gil. High-Performance Nanosensors Based on Plasmonic Fano-like Interference: Probing Refractive Index with Individual Nanorice and Nanobelts. ACS Nano 6 (2012) 8989.
- [4] B. Luk'yanchuk, N. I. Zheludev, S. A Maier, N. J. Halas, P. Nordlander, H. Giessen, C. T. Chong. The Fano resonance in plasmonic nanostructures and metamaterials. Nature Mater. 9 (2010) 707.
- [5] V. Giannini, Y. Francescato, H. Amrania, C. C. Phillips, S. A. Maier. Fano resonances in nanoscale plasmonic systems: a parameter-free modeling approach. Nano Lett. (2011) 2835.
- [6] N. Verellen et al., 2014 (submitted).