

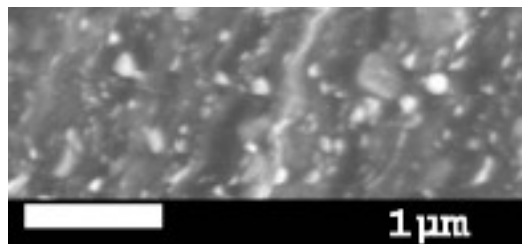
## NANOPARTICLES OF IRON OXIDES INCREASED MAGNETIZATION VALUES

**Pedro Vera-Serna<sup>1\*</sup>, Iván Ricardo Barajas-Rosales<sup>1</sup>, Felipe Nerhi Tenorio.González<sup>1</sup>**

<sup>1</sup> *Universidad Politécnica de Tecámac, Prolongación 5 de mayo No 10, C.P. 55740, Tecámac, Estado de México, México.*

\*pedro\_verasr@uptecamac.edu.mx

The advanced materials are researched and applied on the world in communications devices, other studies as possible candidates to use in energy efficient derivate nanoscience experiments and studies, nanoelectronics devices, high frequency electronic components, high-performance permanent or hard magnets, products with applications on magnetic data storage media, magnetic refrigerants, magnetic random access memory devices and spin logic devices, others as hyperthermia, nanoparticles for biomedical applications, delivery and controlled release of drug molecules between others [1,2,3,4]. During 10 years have been developed studies based on Iron Oxides using high energy miller and the experiments were developed using X Ray Diffraction, Scanning Electron Microscopy, Particle Size Analysis and Magnetometry. The materials when are exposed a magnetic field it has different response on hysteresis cycle, the results shown in products based on iron oxides and ferrites that when decrease the particle size to nanometers scale magnetization increase, in different cases were observed the magnetization with milling process, some materials have new crystalline structure on ceramics and on other cases the crystal structure still without change but with values higher than material with particle size superior to 500nm, on microscopy were detected particles under 100 nm.



**Figure 1** – Nanometric ceramic

**Key Words:** Nanomaterials, Nanoparticles, Magnetic Materials, Advanced Ceramics

### References

- [1] S.S., *et al.*, *J. Magn. Magn. Mater*, **522**, 1167550, (2021).
- [2] M.V., *et al.*, *J. Magn. Magn. Mater*, **522**, 167570, (2021).
- [3] D.T.N., *et al.*, *J Anal Methods Chem*, **5576283**, 1-7, (2021).
- [4] M.S., *et al.*, *Appl. Phys. A.*, **125**, 226, (2019).

## EXPERIMENTAL APPROACHES IN NANOMEDICINE AND IMMUNOTHERAPIES FOR CANCER THERAPEUTICS

**Antonio TOPETE<sup>1\*</sup>**, Rossina DOMÍNGUEZ<sup>1</sup>, Dante SÁNCHEZ<sup>1,2</sup>, Noé ROSAS<sup>1</sup>, Edith LOZANO<sup>1</sup>, Adrián VILLANUEVA<sup>1</sup>, Rublee SEVILLA<sup>1</sup>, Josué JUÁREZ<sup>3</sup>, Natalia HASSAN<sup>4</sup>, Alicia DEL TORO<sup>1</sup>, Antonio QUINTERO<sup>1</sup>, Adrián DANERI<sup>1</sup>

<sup>1</sup> CUCS-Universidad de Guadalajara, Sierra mojada 950, C.P. 44230, Guadalajara, Jalisco, México.

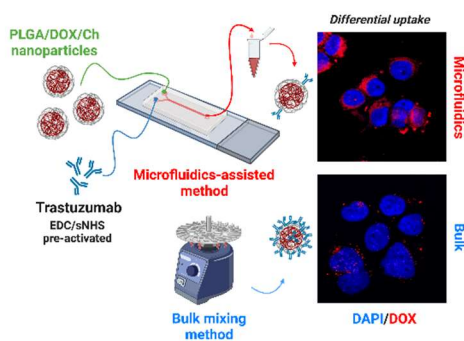
<sup>2</sup> Universidad Tecnológica de Jalisco, Luis Jiménez 577, C.P. 44979 Guadalajara, Jalisco, México.

<sup>3</sup> Departamento de Física, Universidad de Sonora, Unidad Centro, Hermosillo, Sonora, 83000, México.

<sup>4</sup> Programa Institucional de Fomento a la I+D+i, Universidad Tecnológica Metropolitana, San Joaquín, P. O. Box 2409, Chile.

\*antonio.topete@cucs.udg.mx

Nanotechnology applied to human healthcare, called nanomedicine, has been the source of numerous novel approaches for the treatment of different types of cancer. Nanocarrier-based therapeutic has allowed to reduce the toxic side effects of standard chemotherapeutics, and, in specific cases, to improve the therapeutic performance of drugs in solubilized forms. Besides drug transport and delivery, optically activated therapies based on gold and fluorochrome-polymer nanoparticles are also a new strategy to treat tumors in a time-space controlled manner [1]. On the other hand, immunotherapies have recently gained a lot of interest due to their astonishingly positive results on specific cancers [2]. In this talk, we will review the basis of photoactivatable nanoparticles prepared by wet-chemical synthesis methods and the attempt of our group to harness the immunological system to enhance the antitumoral response of combined therapies.



**Key Words:** Cancer, hollow gold nanoshells, nanomedicine, phototherapies, immunotherapies.

### References

[1] Luo, D., et al. *Adv. Sci.* **4**, 1600106-n/a, (2017).

[2] Irvine, J.D., et al. *Nat. Rev. Immunol.* **20**, 321-334, (2020).

## Influence on the optoelectronic properties of alkaline metal-doped tantalum pentoxide from first principles

S. Marin-Silva<sup>a</sup>, I. Perez<sup>b</sup>

<sup>a</sup> Departamento de Física y Matemáticas, Instituto de Ingeniería y Tecnología, Universidad Autónoma de Ciudad Juárez, Ave. Del Charro # 450 Nte. C.P. 32310, Cd. Juárez, Chihuahua, México.

<sup>b</sup>National Council of Science and Technology, Departamento de Física y Matemáticas, Instituto de Ingeniería y Tecnología, Universidad Autónoma de Ciudad Juárez, Ave. Del Charro # 450 Nte. C.P. 32310, Cd. Juárez, Chihuahua, México

\*al198610@alumnos.uacj.mx

The Ta<sub>2</sub>O<sub>5</sub> has direct gap band of 4 eV and is a semiconductor material used for many applications such as electrochromic devices in smart windows. In the present work we studied the effect of doping using alkaline metals (MA: Li, Na, K) on the structure of the β-Ta<sub>2</sub>O<sub>5</sub> phase and γ-Ta<sub>2</sub>O<sub>5</sub> phase with several concentrations of MA. The methodology proposal was the construction of a super cell that later made the geometric optimization to obtain the convergence in the CASTEP program getting the optoelectronic properties and coloration efficiency (CE) to wavelengths in the range from 550 nm to 637 nm. The calculations were realized with DFT (Density Functional Theory).

**Key words:** Ta<sub>2</sub>O<sub>5</sub>, Optoelectronics, Doping, DFT, Properties.

### References

- [1] B.R. Sahu et al., *Theoretical study of structural and electronic properties of β-Ta<sub>2</sub>O<sub>5</sub> and δ-Ta<sub>2</sub>O<sub>5</sub>*, *The American Physical Society*, 1-6, ( 2004).
- [2] V.A S., et al., *Electronic structure and charge transport properties of amorphous Ta<sub>2</sub>O<sub>5</sub>*, *Journal of Non-Crystals Solids*, **354.**, 3025-3033, ( 2008).
- [3] M. V. Ivanov, T. V. Perevalov, V. Sh. Aliev et al., *Ab Initio Simulation of the Electronic Structure of δ-Ta<sub>2</sub>O<sub>5</sub> with Oxygen Vacancy and Comparison with Experimental*, *Journal of Experimental and Theoretical Physical*, **6**, 1035-1040, (2011).
- [4] V. Ivanov Maxim, V. Timofey et al., *Electronic structural of δ-Ta<sub>2</sub>O<sub>5</sub> with oxygen vacancy: ab initio calculations and comparison with experiment*, *Journal of Applied Physical*, **110**, 1-5, (2011).

## MoS<sub>2</sub> NANOPARTICLES CORE SHELL SYNTHESIZED BY FEMTOSECOND LASER ABLATION OF SOLIDS IN LIQUIDS

**Mariela Flores Castañeda<sup>1</sup>, Italia Martin Del Campo Rizzuto<sup>2</sup>, Santiago Camacho López<sup>3</sup>**

<sup>1</sup>*Departamento de Óptica, Centro de Investigación Científica y de Educación Superior de Ensenada, Carr. Tijuana-Ensenada 3918, Zona Playitas, 22860 Ensenada, B.C.*

<sup>1</sup>*Departamento de Biomedicina, Centro de Investigación Científica y de Educación Superior de Ensenada, Carr. Tijuana-Ensenada 3918, Zona Playitas, 22860 Ensenada, B.C.*

\*Corresponding author mar.floc@hotmail.com.

The MoS<sub>2</sub> nanoparticles were synthesized using femtosecond laser ablation of solids in liquids technique, starting a MoS<sub>2</sub> target with a purity of 99.99%, the liquid media were ethanol, ethanol-glycerol mixture at different concentrations. MoS<sub>2</sub> nanoparticles have been frequently used as carriers for loading and delivering of cancer therapeutic agents due to their biocompatibility, insolubility, estability, superficial area, etc. In this work alpha lipoic acid (ALA) was used for the functionalization of the nanoparticles, the ALA was solubilized in ethanol and a ethanol: glycerol mixture 80:20 and this solution was used as a medium for the ablation. The composition, stability and morphology of the nanoparticles was studied by spectrometry micro-Raman, UV-Vis spectrophotometry and transmission electron microscopy, the morphology obtained was a core shell spherical and hexagonal nanoparticles, the Raman spectra shows 2 bands corresponding to MoS<sub>2</sub> without oxides presence, the shell is attributed at carbon from ethanol.

- [1] Yang H, Zhao J, Wu C, Ye C, Zou D and Wang S 2018 Facile synthesis of colloidal stable MoS<sub>2</sub> nanoparticles for combined tumor therapy *Chem. Eng. J.* **351** 548–58
- [2] Huang Z, Qi Y, Yu D and Zhan J 2016 Radar-like MoS<sub>2</sub> nanoparticles as a highly efficient 808 nm laser-induced photothermal agent for cancer therapy *RSC Adv.* **6**
- [3] Wang J, Li Z, Yin Y, Liu H, Tang G, Ma Y, Feng X, Mei H, Bi J, Wang K and Chen Z 2020 Mesoporous silica nanoparticles combined with MoS<sub>2</sub> and FITC for fluorescence imaging and photothermal therapy of cancer cells *J. Mater. Sci.* **55**

## The MoS<sub>2</sub>: A Hybrid Solar Cell Prototype

Manuel Ramos<sup>1,\*</sup>

1) Departamento de Física y Matemáticas, Instituto de Ingeniería y Tecnología, Universidad Autónoma de Cd. Juárez, Avenida del Charro 450 N, Cd. Juárez, Chihuahua, C.P. 32310, México.

\*corresponding author: manuel.ramos@uacj.mx

### Abstract

The Molybdenum Disulfide (MoS<sub>2</sub>) have been studied with intensity in the past 20 years, its chemical structure was first reported by Linus Pauling, proposing a series of two-dimensional sheets stacked by weak van der Waals interaction. Later, the mineral was first used as lubricant to avoid the wear/tear of mechanical parts, and as “workhorse” in catalytic procedure known as hydrodesulphurization of crude oil and recently in the field of nanoelectronics. This talk will present a comprehensive panorama of the exceptional properties of this low dimension material, with special emphasis in the electronic structure when interacts with indium-tin-oxide (ITO) by theoretical and experimental data from RF-sputtering deposits of ITO-MoS<sub>2</sub> thin films (~100nm-300nm), I-V curves, atom probe tomography, scanning and transmission electron microscopy and density functional theory calculations. Results, Results, <110>-orientation are aligned perpendicular to the ITO film with principal reflections at (002), (100), (101), (201), APT reveals MoS<sup>+2</sup>, MoS<sup>+3</sup> as major evaporated molecular ions and indicates no significant diffusion/segregation of Mo or S species within ITO layer. Density functional theory calculations indicate ITO and MoS<sub>2</sub> conform a Schottky barrier due to *d*-orbital interactions creating an ohmic contact and the combination of transparent ITO and semiconducting MoS<sub>2</sub> can produce an efficiency of 2.48% for our proposed hybrid organic-semiconductor solar cell prototype.

**Keywords:** MoS<sub>2</sub>, Thin Film, APT, Microscopy, Electron

### References:

- [1] Manuel Ramos *et al.*, “**Mechanical properties of RF-sputtering MoS<sub>2</sub> thin films**”, Surf. Topogr.: Metrol. Prop. 5 (2017) 025003.
- [2] Ramos M. *et al.*, USPTO #10727428 (2020/7/28).
- [3] Manuel Ramos *et al.* “**Study of indium tin oxide–MoS<sub>2</sub> interface by atom probe tomography**”, MRS Communications, (2019), 1 of 6. doi:10.1557/mrc.2019.150
- [4] López-Galán *et al.*, MRS Comm. (Under review) 2021.

## Plasmonic biosensor for SARS-CoV-2 detection.

Juan-Pablo CUANALO-FERNÁNDEZ<sup>1\*</sup>, Svetlana MANSUROVA<sup>1</sup>, Rubén RAMOS-GARCÍA<sup>1</sup>, Alejandro REYES-CORONADO<sup>2</sup>, Nikolai KORNEEV<sup>1</sup>, Ismael COSME-BOLAÑOS<sup>1</sup>, María-Beatriz DE-LA-MORA-MOJICA<sup>3</sup>, Teresita SPEZZIA-MAZZOCO<sup>1</sup>, Jonathan-Alexis URRUTIA-ANGUIANO<sup>2</sup>, Selma-Flor GUERRA-HERNÁNDEZ<sup>1</sup> y Cristina DÍAZ-FAILACH<sup>1</sup>.

<sup>1</sup>Departamento de Óptica, Instituto Nacional de Astrofísica, Óptica y Electrónica, CP 72840, Puebla, México.

<sup>2</sup>Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, Ciudad Universitaria, Av. Universidad 3000, CP 04510, Ciudad de México, México.

<sup>3</sup>Departamento de micro y nanotecnologías, Instituto de Ciencias Aplicadas y Tecnología, Universidad Nacional Autónoma de México, CP 04510, Ciudad de México, México.

[\\*juancuanalo@inaoe.mx](mailto:juancuanalo@inaoe.mx)

A biosensor is a device able to transform a biological signal into an electrical signal; among the different approaches of biosensing systems, those that are based on surface plasmon resonance (SPR) and localized surface plasmon resonance (LSPR) are particularly attractive for detecting different classes of analytes of clinical interest [1]. Typically, plasmon excitation is detected as an abrupt decline in reflectivity above the critical angle. Due to biological compatibility, gold is an ideal metal to generate a plasmonic field (penetration depth ~100-500 nm) that is sensitive to perturbations in volume and events that occur near the surface, eg hybridization events [2]. In this work, we present the development of the prototype of an optical biosensor capable of detecting the SARS-CoV-2 virus in two modalities, SPR and LSPR. In both cases we use an interferometric method [3] to measure a phase-shift around the plasmon resonance. The gold nanofilm (SPR) or the gold nano-islands (LSPR) were functionalized with thiolate oligonucleotides complementary to specific regions of the genetic material of the SARS-CoV-2. Experimental results demonstrate the functionalization of the gold nano film in situ.

The proposed biosensor exhibits high sensitivity towards selected SARS-CoV-2 sequences with a limit of detection in concentration around 10nM (under laboratory conditions) and allows specific detection in a multigene mixture.

**Key Words:** Biosensor; Surface Plasmonic Resonance; SARS-CoV-2; gold nano-islands.

### References

- [1] A. J. Haes, et al. J. Am. Chem. Soc., vol. 127, no. 7, pp. 2264, Feb. (2005).
- [2] G. Qiu et al., S Nano, p. acsnano.0c02439, Apr. (2020).
- [3] G. Qiu et al., Opt. Lett., vol. 40, no. 9, p. 1924, May (2015).

# OPTICAL EFFICIENCIES OF 2D HONEYCOMB-LIKE ARRAYS OF Ag NANOPARTICLES

A. Ramos Romero<sup>1</sup> and A. L. González<sup>2</sup>

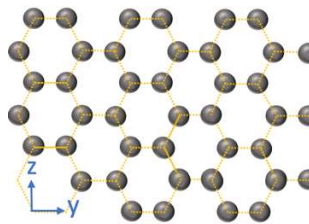
<sup>1</sup> *Facultad de Ciencias Físico-matemáticas, Benemérita Universidad Autónoma de Puebla, Puebla, Puebla, 72592, México.*

<sup>2</sup> *Instituto de Física, Benemérita Universidad Autónoma de Puebla, Apartado Postal J48, 72570 Puebla, México*

\*anagr@ifuap.buap.mx

Periodic 2D systems of plasmonic Ag nanoparticles (Ag NPs) are of great interest because of the wide range of applications as SERS substrate, for light trapping, and others. Besides, several actual techniques allow their controlled fabrication [1,2]. Herein, we have studied a specific geometry, the Ag NPs are arranged forming a kind of graphene layer or 2D honeycomb, see Figure 1. We have used the Discrete dipole approximation [3] to calculate the extinction, absorption and scattering optical efficiencies varying the lattice parameter and the diameter of the NPs when embedded in a SiO<sub>2</sub> solid matrix.

It is well known that for an isolated Ag NP with a radius smaller than 10 nm, the scattering is null, therefore  $Q_{\text{ext}}=Q_{\text{abs}}$ . However, our simulations indicate that for the periodic array the absorption and scattering contributions to the extinction are different from those observed in a single NP, being in general  $Q_{\text{ext}}\neq Q_{\text{abs}}$ . Besides, we have also identified the plasmonic modes and give an interpretation of their origin.



**Figure 1** –Honeycomb-like periodic array of Ag NPs. The electric field impinges perpendicular to the yz plane.

**Key Words:** honeycomb-like arrays, silver nanoparticles, optical efficiencies, discrete dipole approximation.

## References

- [1] S. Mookapati, F. J. Beck, A. Polman and K. R. Catchpole, Appl. Phys. Lett. **95**, 053115 (2009)
- [2] T. D. Corrigan, S. Guo, R. J. Phaneuf, and H. Szmazinski, J. of Fluorescence, **15**, 5, 777-784( 2005)
- [3] B. T. Draine and P. J. Flatau, J. Opt. Soc. Am. A, **25**,11, 2693-2703 (2008)

## **Theoretical Study on the Cl-Au-P- (CH)<sub>n</sub> gold complexes.**

**Pedro Francisco-Santiago**

**Facultad de Ciencias, Departamento de Física-UNAM**  
**Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León.**  
[peter@ciencias.unam.mx](mailto:peter@ciencias.unam.mx)

In this work we study the electronic emission and absorption processes occurring in Cl-Au-P-(CH)<sub>n</sub>-type Gold complexes using the Time-dependent Density Functional Theory (TD-DFT) as methodology, within the scalar relativistic and spin orbit approximations. We have analyzed these electronic processes by applying the Kasha rules, which has allowed us to describe and understand the singlet and triplet transitions, which give rise to the luminescence and phosphorescence processes observed in these gold complexes [1]. It should be noted that due to their photophysical properties, these compounds have been proposed to be used as biological markers.

[1] Polyhedron 179 (2020) 114262