



# Annealing Effects on the Interband Transition and Optical Constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) Nano Thin Films in Cancer Cells, Tissues and Tumors under Synchrotron and Synchrocyclotron Radiations

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### Annealing Effects on the Interband Transition and Optical Constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) Nano Thin Films in Cancer Cells, Tissues and Tumors under Synchrotron and Synchrocyclotron Radiations

Alireza Heidari<sup>1,2,3,4\*</sup>, Margaret Hotz<sup>1,2,3</sup>, Nancy MacDonald<sup>1,2,3</sup>, Victoria Peterson<sup>1,2,3</sup>, Angela Caissutti<sup>1,2,3</sup>, Elizabeth Besana<sup>1,2,3</sup>, Jennifer Esposito<sup>1,2,3</sup>, Katrina Schmitt<sup>1,2,3</sup>, Ling-Yu Chan<sup>1,2,3</sup>, Francesca Sherwood<sup>1,2,3</sup>, Maria Henderson<sup>1,2,3</sup> and Jimmy Kimmel<sup>1,2,3</sup>

<sup>1</sup>Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA

<sup>2</sup>BioSpectroscopy Core Research Laboratory, California South University, 14731 Comet St. Irvine, CA 92604, USA

<sup>3</sup>Cancer Research Institute (CRI), California South University, 14731 Comet St. Irvine, CA 92604, USA

<sup>4</sup>American International Standards Institute, Irvine, CA 3800, USA

**\*Corresponding Author:** Alireza Heidari, Faculty of Chemistry, California South University, 14731 Comet St. Irvine, CA 92604, USA, Email: [Scholar.Researcher.Scientist@gmail.com](mailto:Scholar.Researcher.Scientist@gmail.com); [Alireza.Heidari@calsu.us](mailto:Alireza.Heidari@calsu.us); [Central@aisi-usa.org](mailto:Central@aisi-usa.org)

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#### Abstract

In the current research, annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations is investigated. The calculation of thickness and optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations produced using sol-gel method over glassy medium through a single reflection spectrum is presented. To obtain an appropriate fit for reflection spectrum, the classic Drude-Lorentz model for parametric di-electric function is used. The best fitting parameters are determined to simulate the reflection spectrum using Lovenberg-Marquardt optimization method. The simulated reflectivity from the derived optical constants and thickness are in good agreement with experimental results.

**Keywords:** Annealing, Interband Transition; Optical Constants; Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>); Nano Thin Films; Cancer Cells; Tissues and Tumors; Synchrotron and Synchrocyclotron Radiations



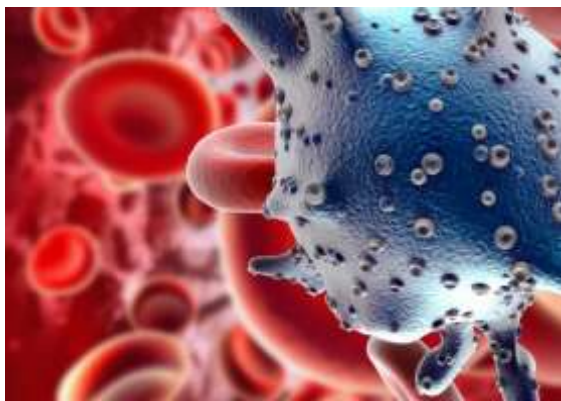
# Annealing Effects on the Interband Transition and Optical Constants of Ruthenium (IV) Oxide ( $\text{RuO}_2$ ) and Ruthenium (VIII) Oxide ( $\text{RuO}_4$ ) Nano Thin Films in Cancer Cells, Tissues and Tumors under Synchrotron and Synchrocyclotron Radiations

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Annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide ( $\text{RuO}_2$ ) and Ruthenium (VIII) Oxide ( $\text{RuO}_4$ ) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations.

## Introduction

Annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide ( $\text{RuO}_2$ ) and Ruthenium (VIII) Oxide ( $\text{RuO}_4$ ) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations is investigated. Ruthenium (IV) Oxide ( $\text{RuO}_2$ ) and Ruthenium (VIII) Oxide ( $\text{RuO}_4$ ) is a semi-conductor of type n which its 3d level is filling up [1-67] and it belongs to a group of smart materials that reacts to variations of temperature, electrical or magnetic fields and pressure. This oxide can be used as thin films for a wide range of applications including electrical and or optical-thermal switching tools and energy

storing covers [67-103]. Therefore, determining optical constants (refractive coefficient,  $n$ , and extinction coefficient,  $k$ ) of Ruthenium (IV) Oxide ( $\text{RuO}_2$ ) and Ruthenium (VIII) Oxide ( $\text{RuO}_4$ ) thin films is essential for designing optoelectrical and optical tools for producing optical covers and similar tools such as multilayer covers and filters [104-184]. The measured experimental parameters including optical reflectivity are used as a function of wavelength to determine optical parameters of thin layers [185-257]. For determining optical parameters, various physical models such as Kuschi, Frouhi-Blumber and Tawk-Lorentz have been suggested to calculate refractive coefficient,  $n$ , and extinction coefficient,  $k$ , for any thin layer, an appropriate optical model should be selected and used for estimation of real and imaginary di-electric function according to its physical condition [258-313]. To do this, an initial guess is needed for parameters of di-electric function and thickness which is defined as a range regarding physical characteristics of thin film and the available results in the literature. Ruthenium (IV) Oxide ( $\text{RuO}_2$ ) and Ruthenium (VIII) Oxide ( $\text{RuO}_4$ )-annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide ( $\text{RuO}_2$ ) and Ruthenium (VIII) Oxide ( $\text{RuO}_4$ ) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations are produced over glassy medium in sol-gel laboratory, Faculty of Chemistry, BioSpectroscopy Core Research Laboratory and Cancer Research Institute (CRI) at California South University, Irvine, California, USA, under similar conditions. Measurement of thin films are



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performed on four samples of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) as annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations with mole ratio of 0.5, 1 and 1.5% of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) [314-467]. Simulation of experimental spectra are performed using a single reflection spectrum of thin films and through Drude-Lorentz physical model in optimization process of Lovenberg-Marquardt. Optical constants such as reflection coefficient, n, extinction coefficient, k, and layer thickness are simultaneously determined at wavelength of 400-1100 (nm).

## Modeling, Simulation and Calculation Method

A usual method for describing optical constants of thin films is utilizing classic dispersion relationships based on di-electric function. One of the oldest and most applicable dispersion relationships is Drude-Lorentz di-electric equation which is based on the interaction between light and material. This relationship is shown in Eq. (1):

$$\varepsilon = \varepsilon_{\infty} + \sum_{j=1}^n \frac{f_j E_{0j}^2}{E_{0j}^2 - E^2 + i\Gamma_j E} + \frac{E_p^2}{E^2 + iE_{\tau} E} \quad (1)$$

Where  $\varepsilon_{\infty}$ ,  $f_j$ ,  $E_0$  and  $\Gamma_j$  are di-electric constant at high frequencies, resonance amplitude, power and resonance width-band which are recognized as the reason for damping. Damping is due to absorption process which includes transition between two states. The third term is related to Drude model.  $E_p$  is density of Plasma energy and  $E_{\tau}$  is incident energy [4]. The complex di-electric function as  $\varepsilon = \varepsilon_1 + i\varepsilon_2$  which describes the reaction of material with electromagnetic waves as a

function of photon energy, E, or wavelength,  $\lambda$ , has a real part  $\varepsilon_1$  and an imaginary part  $\varepsilon_2$ . Real and imaginary parts of complex reflection coefficient, namely n ( $\lambda$ ) and k ( $\lambda$ ) are related to di-electric function as Eq. (2) [5]:

$$n(\lambda) = \left( \frac{\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2}}{2} \right)^{1/2} \quad (2)$$

$$k(\lambda) = \left( \frac{-\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2}}{2} \right)^{1/2}$$

Reflection spectrum (R) of samples for normal incident is a function of film thickness d, medium reflection coefficient S, incident light wavelength  $\lambda$ , reflection coefficient n( $\lambda$ ) and extinction coefficient k( $\lambda$ ).

Simulation of the measured reflection data using optimization of objective function, which is the square of difference between the measured reflection spectrum and the calculated one, is defined as:

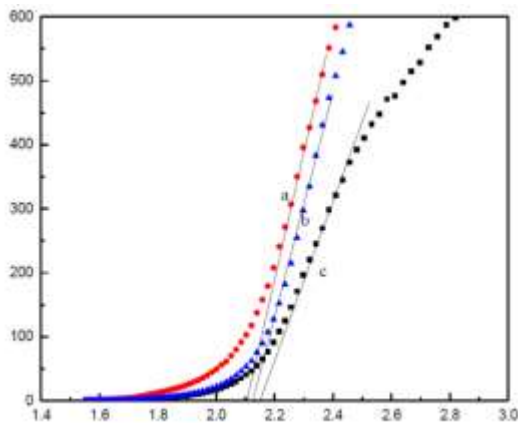
$$O = (\varepsilon_{\infty}, f, \Gamma, E_0, E_p, E_{\tau}, d) = \sum (R_{meas} - R_{calc})^2 \quad (3)$$

Where,  $R_{meas}$  and  $R_{calc}$  are the measured and theoretical reflection spectrum, respectively. using the fitting parameters obtained from minimization of objective function, dispersion curves of reflection and extinction coefficients can be estimated.

## Results and Discussion

The measured and simulated reflection spectra with fitting parameters of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>)-annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations at various concentrations of 0.5, 1 and 1.5%, named as a, b, and c, and annealing effects on the interband

transition and optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations sample, named as p, are shown in Figure (1) in wavelength range of 400-1100 (nm) (visible regions close to infrared) using Drude-Lorentz model for air, film, medium, air system.



**Figure 1:** Results of simulating the reflection spectrum for Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>)-annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations at concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) non-doped.

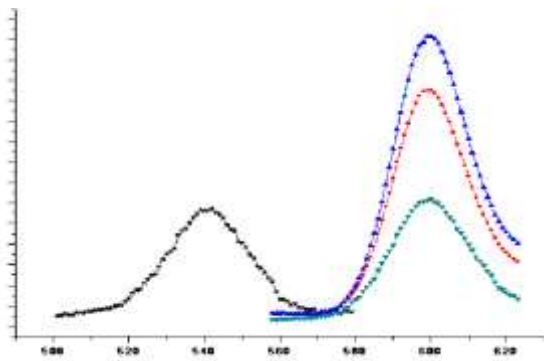
Comparison of the results were shown that the sample containing 0.5% of Ru (sample a) has shown more reflectivity than samples containing 1% and 1.5% of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) (samples b and c). As can be seen in Figure (1), the reflection of thin films is decreased by increase in mole concentration of Ru to Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>). This reduction can be attributed to various reasons such as increasing roughness, increasing

thickness and increasing the concentration of contaminant. The results of investigation about surface roughness using AFM method confirms the increasing of roughness by increasing the concentration of Ru. Therefore, dispersion of incident light is increased in thin films. Variation of thickness of thin film by increasing the percentage of Ru is effective in variation of reflectivity of thin films which is due to sol viscosity. Changing the crystalline structure and chemical composition of thin films induced by penetration of Ru ions into the crystalline lattice of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) is another effective factor which leads to changing the reflection spectrum. The results of structural analysis using XRD confirms the tendency to be amorphous by increasing the concentration of contaminant. The best fitting parameters obtained from optimization process and experimental data fitting are listed in Table (1).

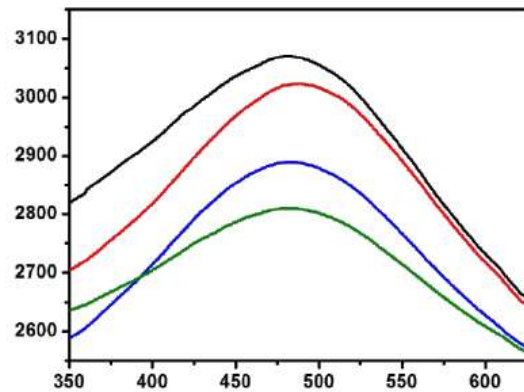
**Table 1:** Fitting parameters of di-electric function of DL model.

Parameter	Pure	% 0.5 Ruthenium (IV) Oxide (RuO <sub>2</sub> ) and Ruthenium (VIII) Oxide (RuO <sub>4</sub> )	1% 1 Ruthenium (IV) Oxide (RuO <sub>2</sub> ) and Ruthenium (VIII) Oxide (RuO <sub>4</sub> )	% 1.5 Ruthenium (IV) Oxide (RuO <sub>2</sub> ) and Ruthenium (VIII) Oxide (RuO <sub>4</sub> )
$\epsilon_{\infty}$	4.4	3.4	2.4	1.4
$E_p$	1.84	1.74	1.64	1.54
$E_{\tau}$	0.44	0.43	0.34	0.24
$f$	0.34	0.24	0.14	0.04
$E_0$	2.1	1.9	1.8	1.7
$\Gamma$	0.4	0.3	0.2	0.1
$d (nm)$	205	305	405	505

As can be seen in Table (1), more increase in Ru leads to increase in  $\Gamma$ ,  $f$ ,  $E_0$  and  $d$  and decrease in other parameters as crystalline structure and inter-atom distance changes in lattice of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) thin film. According to [7],  $E_0$  in the range of 2.9-3.1 (eV) shows optical transition capacity band to displaced state of conducting band which according to the data of Table (1), it can be concluded that optical transition energy (gaff energy) increases with increase in Ru concentration. The calculation results of optical constants including reflection coefficient and extinction coefficient using the parameters of obtained di-electric function from the optimization process of thin films at various concentrations of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) as 0.5% (sample a), 1% (sample b) and 1.5% (sample c) are shown in Figures (2) and (3), respectively.



**Figure 2:** Reflection coefficient of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) thin films with Ru concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) pure sample.



**Figure 3:** Extinction coefficient of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) thin films with Ru concentrations of (a) 0.5%, (b) 1%, (c) 1.5% and (p) pure sample.

As can be seen in Figure (2), reflection coefficient of samples at 500-1100 (nm) are the same and are decreased by increasing wavelength. By increasing the concentration of Ru, reflection coefficient is totally reduced which is in good agreement with the results related to variations of reflectivity in Figure (1) in which, increasing roughness leads to increase in dispersion and hence, reducing the amount of reflection spectrum. It can be seen in Figure (3) that  $k(\lambda)$  for two samples of p and a are of increasing rate at wavelength range of 400-500 (nm). Further, all samples are of decreasing rate at the range of 500-800 (nm). Totally,  $k(\lambda)$  is reduced by increase in Ru concentration. In other words, optical absorption is reduced in this range and the emerged peaks at extinction coefficient are in agreement with parameters of Drude-Lorentz obtained from the optimization algorithm.

### Conclusions, Summary, Recommendations, Perspectives, Useful Suggestions and Future Studies

The results of optimization algorithm of Lovenberg-Marquardt with physical model of



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Drude-Lorentz for determining optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>)-annealing effects on the interband transition and optical constants of Ruthenium (IV) Oxide (RuO<sub>2</sub>) and Ruthenium (VIII) Oxide (RuO<sub>4</sub>) nano thin films in cancer cells, tissues and tumors under synchrotron and synchrocyclotron radiations produced using sol-gel method through a single reflection spectrum show that higher doping leads to lower reflectivity and reflection coefficient and also, leads to increase in thickness of thin layer.

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## Authors' Brief Biographies



Prof. Dr. Alireza Heidari, Ph.D., D.Sc. is a Full Distinguished Professor and Academic Tenure of Chemistry and also Enrico Fermi Distinguished Chair in Molecular Spectroscopy at California South University (CSU), Irvine, California, USA. He has got his Ph.D. and D.Sc. degrees from California South University (CSU), Irvine, California, USA. Furthermore, he has double postdocs in Project Management, Oncology, Human Cancer Tissues and Synchrotron Radiation from Monash University, Melbourne, Victoria, Australia and also in Nanochemistry and Modern Molecular Electronic-Structure Computations Theory from California South University (CSU), Irvine, California, USA. His research interests include Biophysical Chemistry, Biomolecular Spectroscopy, Quantum Chemistry, Nanochemistry, Modern Electronic Structure Computations,



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Theoretical Chemistry, Mathematical Chemistry, Computational Chemistry, Vibrational Spectroscopy, Molecular Modelling, Ab initio & Density Functional Methods, Molecular Structure, Biochemistry, Molecular Simulation, Pharmaceutical Chemistry, Medicinal Chemistry, Oncology, Synchrotron Radiation, Synchrocyclotron Radiation, LASER, Anti-Cancer Nano Drugs, Nano Drugs Delivery, ATR-FTIR Spectroscopy, Raman Spectroscopy, Intelligent Molecules, Molecular Dynamics, Biosensors, Biomarkers, Molecular Diagnostics, Numerical Chemistry, Nucleic Acids, DNA/RNA Monitoring, DNA/RNA Hypermethylation & Hypomethylation, Human Cancer Tissues, Human Cancer Cells, Tumors, Cancer Tissues, Cancer Cells, etc. He has participated at more than five hundred reputed international conferences, seminars, congresses, symposiums and forums around the world as yet. Also, he possesses many published articles in Science Citation Index (SCI)/International Scientific Indexing (ISI), Medline/PubMed and Scopus Journals. It should be noted that he has visited many universities or scientific and academic research institutes in different countries such as United States, United Kingdom, Canada, Australia, New Zealand, Scotland, Ireland, Netherlands, Belgium, Denmark, Luxembourg, Romania, Greece, Russia, Estonia, Ukraine, Turkey, France, Swiss, Germany, Sweden, Norway, Italy, Austria, Czech Republic, Hungary, Poland, South Africa, Egypt, Brazil, Spain, Portugal, Mexico, Japan, Singapore, Malaysia, Indonesia, Thailand, Taiwan, Hong Kong, Philippines, South Korea, China, India, Kingdom of Saudi Arabia, Jordan, Qatar, United Arab Emirates, etc. as research fellow, sabbatical and volunteer researcher or visitor and so on heretofore. He has a history of several years of teaching for college students and various disciplines and trends in different universities. Moreover, he has been a senior advisor in

various industry and factories. He is expert in many computer programs and programming languages. Hitherto, he has authored more than twenty books and book chapters in different fields of Chemistry. Syne, he has been awarded more than one thousand reputed international awards, prizes, scholarships and honors. Heretofore, he has multiple editorial duties in many reputed international and peer-reviewed journals, books and publishers. Hitherto, he is a member of more than five hundred reputed international academic-scientific-research institutes around the world. It should be noted that he is currently the President of the American International Standards Institute (AISI), Irvine, California, USA and also Head of Cancer Research Institute (CRI) and Director of the BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



Dr. Margaret Hotz, Ph.D. is the current Junior Postdoctoral Research Fellows under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



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Dr. Nancy MacDonald, Ph.D. is the current Junior Postdoctoral Research Fellows under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



Dr. Angela Caissutti, Ph.D. is the current Junior Postdoctoral Research Fellows under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



Dr. Victoria Peterson, Ph.D. is the current Junior Postdoctoral Research Fellows under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



Dr. Elizabeth Besana, Ph.D. is the current Junior Postdoctoral Research Fellows under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



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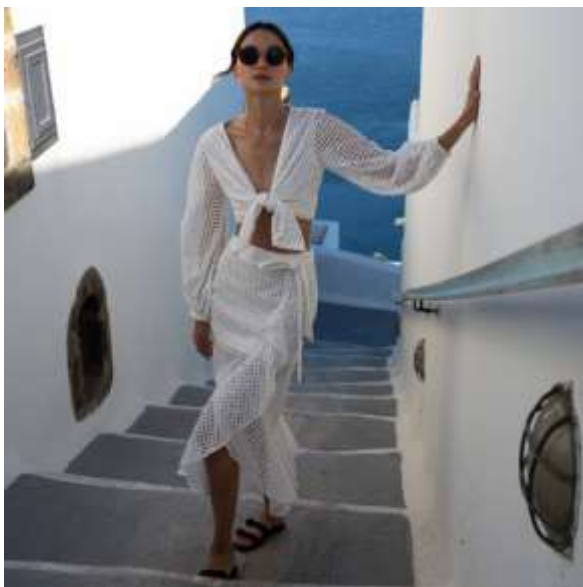
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Dr. Jennifer Esposito, Ph.D. is the current Junior Postdoctoral Research Fellows under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



Dr. Katrina Schmitt, Ph.D. is the current Junior Postdoctoral Research Fellows under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at

California South University (CSU), Irvine, California, USA.



Ling-Yu Chan is a Ph.D. Candidate under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



Francesca Sherwood is a Ph.D. Candidate under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



# Annealing Effects on the Interband Transition and Optical Constants of Ruthenium (IV) Oxide ( $\text{RuO}_2$ ) and Ruthenium (VIII) Oxide ( $\text{RuO}_4$ ) Nano Thin Films in Cancer Cells, Tissues and Tumors under Synchrotron and Synchrocyclotron Radiations

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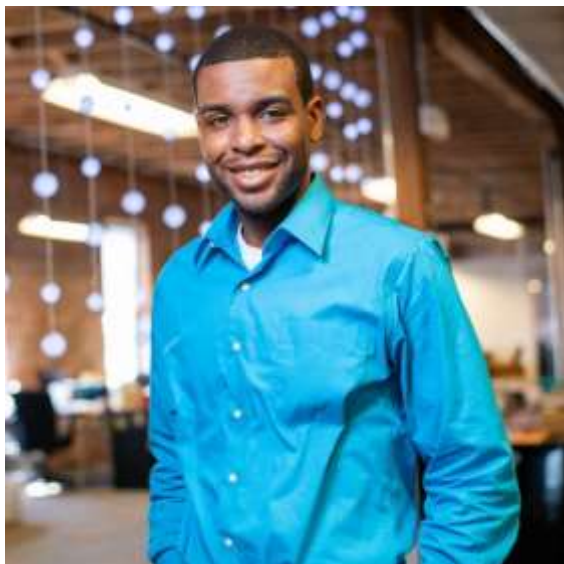
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California South University (CSU), Irvine, California, USA.

Maria Henderson is a Ph.D. Candidate under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at California South University (CSU), Irvine, California, USA.



Jimmy Kimmel is a Ph.D. Candidate under the Supervision of Professor Alireza Heidari at Cancer Research Institute (CRI) and BioSpectroscopy Core Research Laboratory at