## **Eclética Química Journal**

## **Editorial**

On May 18, 2016, the science and technology lost a real giant—José Arana Varela, who passed away at age 72. Describing him as *a giant* does not do justice to the scientist, the professor, the mentor, and the human being. It is with great pleasure that we write the preface to the Eclética Química Journal in honor of Professor José Varela. He was a close colleague, a collaborator, and, above all, a friend for nearly 50 years. This opportunity represents just an excellent excuse to celebrate a most remarkable physicist who has always been far ahead of his time, thanks to a unique combination of scientific visions, creativity, breadth, drive, and dedication. Rather than describing José's distinguished academic career, here we highlight different aspects, which we believe have given it particular impact.

| Vol. 47 | special issue 1 | 2022 |

Varela was born in Martinópolis, São Paulo, Brazil, on April 11, 1944, and left this world in his long-time home of Araraquara, São Paulo. Obviously, a lot of things happened in between, but this editorial is going to focus on the recollections of this giant as seen through his former colleagues and friends. He held a degree in Physics from the University of São Paulo (1968), a Master's degree in Physics from the Instituto Tecnológico de Aeronáutica (1975) and a PhD in Ceramic Materials from the University of Washington (1981). He published over 500 articles in international journals. He developed more than 35 projects and agreements with governments: federal and state and also with companies. He supervised and co-supervised more than 50 theses and dissertations. He received more than 20 awards and honorable mentions, including the Golden Epsilon Award from the Spanish Society of Ceramics and Glass. He worked on a strong exchange with national and international research institutions in Spain, France, USA, Slovenia and Italy. He focused his research in Materials and Metallurgical Engineering, with emphasis on Ceramics, worked mainly on the following topics: thin films, ferroelectric and dielectric materials, varistors, grain boundary properties and sintering.

José Varela was a true innovator who opened numerous new fields of research. A major strength of his scientific approach has always been to precisely demonstrate with rigorous methodologies and simple examples new notions, and to put these notions in much broader perspectives—often inspired by philosophy and arts—to generate paradigms of deep impact. From early works dedicated to sintering and electronic ceramics, to those of us who considered Varela a cherished friend, the fire of science burned brightly within him until the very end. To those of us who considered Varela a cherished friend, the fire of science burned brightly within him until the very end. Many of his colleagues have described him as a force of nature, which indeed he was. He was determined to do cutting edge science each and every day, even toward the end of his life. Amazingly, even several months before his death, at the ripe young age of 71, he was planning on the next project and the meeting with friend to drink a good wine. To his friends and students, Varela will be sorely missed. He was a role model who showed us not only how to be a great scientist but also a wonderful human being. He inspired us by his devotion to his craft and his passion to unlock one of the secrets of nature. He never gave up; he was passionate and truly lived a remarkable life that serves as a shining example to all his colleagues and friends.

Opening this issue the preparation of a W-doped  $Ag_3PO_4$  with high photocatalytic activity by the chemical coprecipitation method and irradiated with a femtosecond laser (FL) is described. A higher structural disorder in the [PO<sub>4</sub>] clusters was observed for the FL irradiated sample ( $Ag_3PO_4$ :W-FL), indicating the formation of Ag metallic from the  $Ag_3PO_4$  structure. The photocatalytic activity of the samples was studied by photodegradation of rhodamine B under visible light irradiation. The formation of Ag nanoparticles on the surface of  $Ag_3PO_4$ :W led to a degradation rate constant 3.54 times higher than the nonirradiated sample. Follow, it is described the catalytic potential of titanium oxide (TiO<sub>2</sub>) and gold doped titanium oxide nanoparticles applied to the selectivity benzyl alcohol oxidation. A composite nanomaterial was obtained with high synergy between gold and TiO<sub>2</sub> nanoparticles, resulting in high catalytic activity for benzaldehyde formation. Selective oxidation of alcohols is one of the most significant transformations of organic chemistry since it is essential for industrial intermediates production. The next article describes the synthesis of YVO<sub>4</sub>:RE (RE = Eu, Tm, and Yb/Er) nanoparticles using the microwave-assisted hydrothermal method. Different characterization techniques have been employed to examine the structural, optical,

as well as its morphology and the photoluminescence (PL) emissions. The as-synthesized samples present different emission colors due to RE<sup>3+</sup> ions, as well as nanosized spherical morphology. These materials are efficient for optical devices. Afterwards, it is presented the quantum chemistry methods used to study a boron nitride nanotube (BNNT) and a carbon nanotube (CNT) as possible carrier agents for the antichagasic benznidazole (BNZ) to improve its water solubility and bioavailability in the organism. For the BNZ@BNNT complex, it was possible to note short interactions, at a distance of 0.215 nm, between hydrogen atoms from BNZ and nitrogen atoms from BNNT. Overall, the results demonstrate that the BNNT is a better candidate to be used as a carrier agent for BNZ than the CNT due to its higher structural and chemical stability, lower binding energy and lower solvation enthalpy. In the sequence, the production of activated carbon (AC) from pumpkin seeds by simultaneous carbonization activation for occupational respiratory protection is described. The AC is derived from carbonaceous sources and used as a technological element for various industrial purposes. Due to this context and to enhance sustainability concepts and human health in the production of materials, this study aimed to produce activated carbon from an abundant agricultural waste in northeast Brazil through a route that not only favors its simultaneous carbonization and activation but also its thermal neutralization, enhancing sustainability concepts and human health in the production of materials. The AC showed yields between 73%-78% and adsorption capacity and selectivity to ammonia gas. The morphology varied in function of the biomass interaction with the type and concentration of acid used. Follow, the readers find a study of surfactant effects in the morphology and the photocatalytic activity of the BaMoO<sub>4</sub> crystals where experimental techniques were applied to investigate the order-disorder degree of samples. The morphologies were investigated by field emission scanning electron microscopy, and the theoretical crystal morphologies were obtained through the Wulff construction. The photocatalytic activity efficiency of the BaMoO<sub>4</sub> crystals were tested against the rhodamine (RhB) dye. BaMoO<sub>4</sub> synthesized with the surfactant sodium dodecyl sulfate presented a monophasic crystal with a disordered structure. The presence of surfactant generated pores on the surfaces of the material that were responsible for the appearance of the adsorptive ability enhancing the adsorption process of the RhB dye in the absence of ultraviolet light. Subsequently, the influence of  $Eu^{3+}$  cations in the host matrix of CaZrO<sub>3</sub> is discussed by analyzing the luminescence and structural properties. The Ca 1-x ZrO<sub>3</sub>:Eu<sub>x</sub> crystals were obtained by a simple sol-gel method followed by a soft thermal treatment without any surfactant. The structural characterization at short-, medium- and long-distance allowed to observe the effect of the dopant in the host matrix. The luminescence profile of the sample was investigated by analyzing the excitation and emission spectrum monitoring the emission at 614 nm and excited at 394 nm, noting that the sample Eu-doped with 0.08 mol% has greater emission intensity. The color variations of the characteristic emissions of Ca 1-x ZrO<sub>3</sub>:Eu<sub>x</sub> crystals were evaluated according to the Commission Internationale de L'Éclairage, observing a red shift for all Eu-doped samples. A general luminescence scheme was proposed combining the density of state and the band structure calculations. Nowadays, the disposal of polluting substances, such as methylene blue (MB) dye, into wastewater, arouses the interest of technologies to remove these pollutants. Here,  $Fe_2O_3$  was obtained by the conventional hydrothermal process and heat-treatment, subsequently FL-irradiated treatment. The mixture of irradiated  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and  $\epsilon$ -Fe<sub>2</sub>O<sub>3</sub> phases revealed lower crystallinity than irradiated  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> samples that together with the increase in crystallinity were crucial to improve the performance of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> irradiated sample in the discoloration of MB, reaching 90% in 75 min of dye solution exposure under UV irradiation. This result was attributed to the increase in active sites due to the density of defects generated, which enhance the degradation process. The next work describes the effect of coupling the Zrmetal-organic frameworks (MOFs) and  $SnO_2$  and its potential for application as photoelectrode in solar cells. Coupling was performed by mechanical mixture followed by heat treatment and the effect of adding two amounts of Zr-MOF (25 and 50 wt%) on morphology and photoelectrochemical properties were investigated. The J-V curves show that the coupling of 25 wt% Zr-MOFs with SnO<sub>2</sub> improves the charge transfer characteristics under light irradiation 1.6 times compared to the pure SnO<sub>2</sub>. Completes this issue the research concerning the modifications of materials for improvement of its photocatalytic activity that has been widely increased due to the potential of heterogeneous photocatalysis for wastewater treatment. One of the most employed methods is the metal doping process into semiconductors, which allows the modification of their electronic structure. As observed by XRD and

Raman results, the Cu insertion into  $TiO_2$  structure induced the stabilization of anatase phase, increasing its content in the samples in relation to the bare  $TiO_2$ . The photoluminescence spectroscopy (PL) results indicated that the Cu insertion into  $TiO_2$  promoted a decrease in the PL emission intensity and a shift of the emission band to the blue region. The photocatalytic activity of the samples for RhB degradation under UV light irradiation indicated that the Cu-doping into  $TiO_2$  led to an enhancement of the photocatalytic activity compared to the bare sample.

## Prof. Dr. Elson Longo (Guest Editor) Prof. Dr. Juan Manuel Andrés Bort (Guest Editor)