# V CINE-CMSC Workshop: Scientific Discussions from $CH_4$ Conversion to Machine Learning Applications (P16-P20)

**São Carlos Institute of Chemistry, University of São Paulo, São Carlos**

**Google Meet (Online Talks) https://meet.google.com/sor-bpkv-dpo**

CENTER FOR INNOVATION ON NEW ENERGIES

Juarez L. F. Da Silva Group

## 06 July 2020 - Module 1: $CH_4$ Conversion to Methanol based on Nanocatalysts and Zeolites.

| Schedule | Talk | Speaker | Institution |
|---|---|---|---|
| 09:00 – 09:20 | **Overview** | Juarez Lopes Ferreira da Silva | IQSC-USP |
| 09:20 – 09:40 | Lanthanum Doped Ceria Shaped Nanostructures for Oxidative Coupling of Methane | Fabiane de Jesus Trindade | UFABC |
| 09:40 – 10:00 | Methane Activation on 3*d* Transition-Metal Clusters $TM_n$ ($n$ = 4 - 15)- The Example of $Fe_n$ | Karla Furtado Andriani | IQSC-USP |
| 10:00 – 10:20 | DFT study of the cleavage of the methane CH bond by $[Cu_2(\mu\text{-}O)]_2^+$ exchanged SSZ-13 zeolite | Sara Figueirêdo de Alcântara Morais | IQ-USP |
| 10:20 – 10:35 | Enhanced Sampling/Molecular Dynamics Methods and QM/MM Technique on the Steric/Electrostatic Effects and Reactivity in Cu-exchanged Zeolite. | Luis Paulo Mezzina Freitas | UNESP |
| 10:35 – 10:50 | An *Ab initio* Investigation of $CH_4$ Dehydrogenation on $(CeO_2)_{10}$ Nanoclusters | Carina de Souza Teixeira Peraça | UFPEL |
| 10:50 – 11:05 | A Theoretical Investigation of $CH_4$ Dehydrogenation on $Co_n$ Nanoclusters ($n$ = 4 - 15) | Priscilla Felício Sousa | IQSC-USP |
| 11:05 – 11:20 | Comparison between hybrid QM/MM and DFT methodologies for the treatment of adsorption over Cu-SSZ-13 zeolite | Bassim Mounssef Junior | IQ-USP |
| 11:20 – 11:35 | Ethane dehydrogenation catalyzed by Ga/SSZ-13 Zeolite | Lucas Welington de Lima | IQ-USP |
| 11:35 – 11:43 | Methane Activation on Zirconium Oxide Nanoclusters | Isabelle Leao Gomes | IQSC-USP |
| 11:43 – 11:51 | Theoretical Study and Development of Metalloenzymes Mimetic for Conversion of $CH_4$ into $CH_3OH$ | Lucas Neres Chagas da Silva | UNESP |

## Informations

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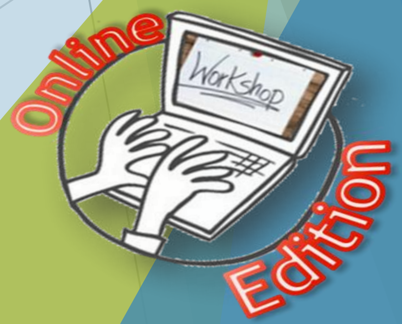

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## 07 July 2020 - Module 2: $CO_2$ Reduction to new products

| Schedule | Talk | Speaker | Institution |
|---|---|---|---|
| 09:00 – 09:20 | Design and Construction of a Differential Electrochemical Mass Spectrometer (DEMS) | Adriana Queiroz | UNICAMP |
| 09:20 – 09:40 | Density Functional Theory Study of the Adsorption of $CO_2$, Alcohols and Additional Model Molecules on Transition-metal Substrates | Paulo de Carvalho Dias Mendes | IQSC-USP |
| 09:40 – 10:00 | Adsorption Site Coordination Effects on the Interaction of $CO_2$ Reduction Intermediates on Cu Substrates. | Lucas Garcia Verga | IQSC-USP |
| 10:00 – 10:15 | How the H co-adsorption and H-OC binding affect the $CO_2$ activation on $Fe_{13}$ cluster? | Vivianne Karina Ocampo Restrepo | IQSC-USP |
| 10:15 – 10:30 | *Ab Initio* Investigation of $CO_2$ Adsorption on 4*d* and 5*d* $TM_8$ Clusters | Matheus Nunes Collacique | IQSC-USP |
| 10:30 – 10:45 | A DFT investigation and comparison of $CO_2$ activation on $(WS_2)_{16}$ with and without Fe adatom | Henrique Alves Bacco Fonseca | IQSC-USP |
| 10:45 – 10:53 | $CO_2$ capture by hybrid materials under electrical potential | Victor Oliveira Valente | UNIFESP |
| 10:53 – 11:08 | Density Functional Theory Investigation of the Adsorption of Methanol, Ethanol and Ethylene Glycol on 3*d*, 4*d*, 5*d* $TM_{15}$ Nanoclusters | Raquel Costabile Bezerra | UFAM |
| 11:08 – 11:28 | The Formation Mechanism of Nano-interfaces between 3*d*-late Transition-metals and $ZrO_2$ Nanoclusters: An *Ab Initio* Investigation | Larissa Zibordi Besse | IQSC-USP |
| 11:28 – 11:36 | Perspectives on NiGa/$ZrO_2$ catalysts for $CO_2$ reduction | Rafael Alves de Sousa | IQSC-USP |
| 11:36 – 11:51 | Theoretical Investigation of the Adsorption of Molecular Probes (CO, $CO_2$, $C_2H_2$, $CH_4$, $H_2$, $H_2O$, $NH_3$, $SO_2$ and $BCl_3$) on the Hydroxyapatite (0001) Surface | Albert Frederico Barbosa Bittencourt | UNICAMP |
| 11:51 – 11:59 | *Ab initio* Investigation of Ligand-protected Binary Copper-Zinc Clusters | Gianluca Ragassi | IQSC-USP |

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## 08 July 2020 - Module 3 : 2D Materials for Photovoltaics Applications

| Schedule | Talk | Speaker | Institution |
|---|---|---|---|
| 09:00 – 09:20 | *Ab initio* Investigation on the Evolution of Physical-Chemical Properties and Formation, Adsorption, and Support Mechanisms of Transition-Metal Dichalcogenides Nanoflakes. | Naidel Antonio Moreira Santos Caturello | IQSC-USP |
| 09:20 – 09:40 | Excitonic Effects on Chalcogenides 2D Materials | Alexandre Cavalheiro Dias | IQSC-USP |
| 09:40 – 10:00 | Electronic Band Alignment and Optical Properties of van der Waals Heterobilayers of Mo, Ni, and Pt Dichalcogenides | Rafael Besse | IFSC-USP |
| 10:00 – 10:15 | Magnetic interaction between $MoS_2$ nanoribbons. | Jean Michel Bracht | UFSCar |
| 10:15 – 10:30 | An *ab initio* investigation of groups III-V 2D monochalcogenides | Mateus Bazan Peters Querne | UFSCar |
| 10:30 – 10:45 | Triangular $MoS_2$ and $MoSe_2$ nanoclusters: a first-principles investigation | Lucas Guilherme Chagas | UFSCar |
| 10:45 – 11:00 | Strain effects on transition metal dichalcogenides heterostructures | João Gabriel Danelon Vieira de Almeida | UFSCar |
| 11:00 – 11:08 | First-principles Investigation of One-atom Monolayer Chalcogenides ($MQ_x$, M = Cu, Ag; $Q$ = S, Se, Te, and $x$ = 0.0 - 2.0) versus Traditional Monolayer Structures. | Guilherme Kazuo Inui | IQSC-USP |
| 11:08 – 11:16 | Role of Adsorption of Atmospheric Molecules on The Electronic Transport Properties of the $MoS_2$ Monolayer | Natan Moreira Regis | UFSCar |

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## 08 July 2020 - Module 4: From 0D to 3D Perovskites Materials for Photovoltaic Applications

| Schedule | Talk | Speaker | Institution |
|---|---|---|---|
| 14:00 – 14:20 | Materials and Processing Development for Highy-efficiency, Stable and Scalable Perovskite Solar Cells | Francineide Araújo | UNICAMP |
| 14:20 – 14:40 | Mixed Halide Lead Free Double Perovskites for Photovoltaic Applications | Julian Francisco Rama Vieira Silveira | IQSC-USP |
| 14:40 – 15:00 | Optical and Dielectric Properties of Lead Perovskite and Iodoplumbate Complexes | Srikanth Malladi | IQSC-USP |
| 15:00 – 15:15 | Experimental and Theoretical Investigation of Novel Low Dimensional Lead-Free Bismuth Based Perovskites | Mailde da Silva Ozório | IQSC-USP |
| 15:15 – 15:30 | Structure-Property Relationships of 27 $ABX_3$ (I-IV-VII) Perovskites | Mariana Candido Gallego | IQSC-USP |
| 15:30 – 15:45 | Scientific Dissemination Using Social Media: Facebook e YouTube | Julia Maria Peixe Santesso | IQSC-USP |

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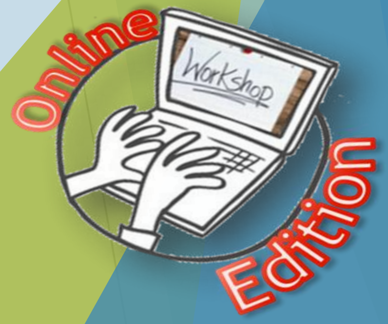

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## 09 July 2020 - Module 5 : Energy Storage using Supercapacitors and Batteries

| Schedule | Talk | Speaker | Institution |
|---|---|---|---|
| 09:00 – 09:20 | Li-air Battery: Electrode design and characterization | Chayene Gonçalves Anchieta | UNICAMP |
| 09:20 – 09:40 | A Complete Ionic Liquid Based Imide Electrolytes Screening for Sodium-ion Batteries: Correlation Between Liquid Nanostructure and $Na^+$ Dynamics | Tuanan da Costa Lourenço | IQSC-USP |
| 09:40 – 09:55 | Comparison between the Performance of Graphene and Graphene Oxide Supercapacitors | Guilherme Ferreira Lemos Pereira | UNIFESP |
| 09:55 – 10:10 | Ether-functionalized Sulfonium Ionic Liquid and its Binary Mixtures With Acetonitrile as Electrolyte for Electrochemical Double Layer Capacitors. | Abner Massari Sampaio | UNIFESP |
| 10:10 – 10:25 | Computational study of confined ionic liquids in $CO_2$ abatement | Rafael Guimarães Pereira | UNIFESP |
| 10:25 – 10:40 | On the behavior of electrical properties of ionic liquids mixtures | Pedro Henrique de Lima Ferreira | UNIFESP |
| 10:40 – 10:48 | *Ab initio* Investigation of Energetic, Structural and Electronic Properties of Sodium Crystals Elements from Groups 14 to 17 | Giovanna Fardini Lima | IQSC-USP |
| 10:48 – 10:56 | Parameterization of Force Fields for Ionic Liquids used in Na and Mg-ion Batteries in the Light of EDA and cDFT Approaches | Letícia Maria Pequeno Madureira | UFSC |
| 10:56 – 11:04 | Computer simulation of aluminate-based ionic liquids as electrolytes for sodium batteries | Rafael Henrique Ratochinski | FFCLRP |
| 11:04 – 11:12 | Mixtures of ionic liquids in coarse-grained model as electrolyte for supercapacitors | Isabel Amaral da Silva | UNIFESP |
| 11:12 – 11:20 | Atomistic simulations of water-in-salt electrolytes in unmodified graphene electrodes | José Amauri Alcântara Lima Junior | UNIFESP |
| 11:12 – 11:28 | MD Simulations of Trialkylsulfonium-Based Ionic Liquids on Nanoporous Graphene Electrodes Models | Matheus Fatorelli Machado | UNIFESP |

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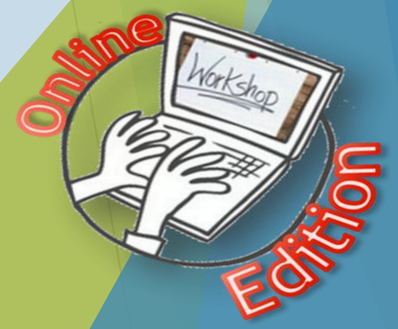

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## 10 July 2020 - Module 6 : Machine Learning Applications in Quantum Chemistry

| Schedule | Talk | Speaker | Institution |
|---|---|---|---|
| 09:00 – 09:20 | Machine Learning Prediction of Nine Molecular Properties Based on the SMILES Representation of the QM9 Quantum-chemistry Dataset | Gabriel Augusto Lins Leal Pinheiro | UNIFESP |
| 09:20 – 09:40 | Machine learning and global optimization algorithms to study the structural and thermal properties of nanoclusters | João Paulo Almeida de Mendonça | IQSC-USP |
| 09:40 – 10:00 | A Feature Engineering Based Strategy to Obtain Insights from Quantum Chemistry Data | Johnatan Mucelini | IQSC-USP |
| 10:00 – 10:20 | Using convolution for molecules properties prediction | Renato Frazzato Viana | UFABC |
| 10:20 – 10:35 | A Bias-Variance Analysis of Machine Learning Models in Quantum Chemistry Data | Luis Cesar de Azevedo | UFABC |
| 10:35 – 11:50 | Clustering methods for selecting representative samples in chemical databases | Felipe Vaiano Calderan | UNIFESP |
| 11:50 – 12:05 | A DFT Investigation of the Physical and Chemical Properties of 8-atom Transition-Metal Clusters - The Case of AlCo Nanoalloys | Felipe Orlando Morais | IQSC-USP |

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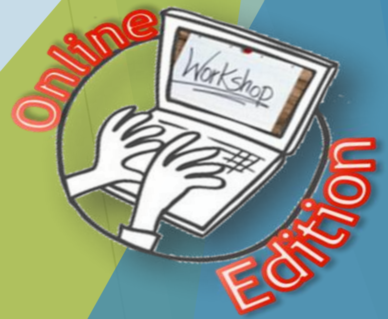

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**10 July 2020 Module 7 :** Evaluation of the Scientific Achievements within the first 24 months
Only for Faculty Members

| Schedule | Speaker | Institution |
|---|---|---|
| 15:00 – 15:20 | Ataualpa Albert Carmo Braga | IQ-USP |
| 15:20 – 15:40 | Gustavo Troiano Feliciano | UNESP |
| 15:40 – 16:00 | Matheus Paes Lima | UFSCar |
| 16:00 – 16:20 | Luís Gustavo Dias | FFCLRP |
| 16:20 – 16:40 | Leonardo José Amaral de Siqueira | UNIFESP |
| 16:40 – 17:00 | Ronaldo Cristiano Prati | UFABC |
| 17:00 – 17:20 | Marcos Gonçalves Quiles | UNIFESP |
| 17:20 – 17:40 | Juarez Lopes Ferreira da Silva | IQSC-USP |
| 17:40 – 18:00 | **Final remarks** | |

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