

**1st Day – September 02, 2019** Chair: Juarez L. F. Da Silva

Location: IQSC - Anfi

Schedule	Description	Speaker	Institution
14:00-14:15	Opening	Emanuel Carrilho	IQSC-USP
14:15-15:00	CMSC Overview	Juarez L. F. Da Silva	IQSC-USP
15:00-16:00	CINE Methane to Products- overview and current status	Fabio Coral Fonseca	IPEN
16:00-16:30	<b>Coffee Break</b>		
16:30-17:30	In operando techniques to unravel reaction mechanism and simultaneous characterization of the catalyst	Pablo Sebastián Fernández	UNICAMP
17:30-18:30	<b>Projects Meeting (CINE - Faculty members)</b>		

**2nd Day – September 03, 2019** Chair: Paulo and Julian

Location: IQSC - Anfi

Schedule	Description	Speaker	Institution
08:30-09:00	DFT Studies of Metallic Nanoparticles Applicable to Heterogeneous Catalysis	Lucas G. Verga	IQSC-USP
09:00-09:30	Molecular Dynamics simulations of ionic liquids of interesting in green technology	Tuanan C. Lourenço	IQSC-USP
09:30-09:50	Computational Design of Novel Carbon Nanotube-based Nanoporous Materials	Julian F. R. V. Silveira	IQSC-USP
10:00-10:30	<b>Coffee Break</b>		
10:30-10:50	Computational Investigation on $M_{13}$ and $M_{14}$ NiGa Ligand Stabilized Binary Nanoclusters, a Novel Class of $CO_2$ Hydrogenation Catalysts	Augusto C. H. da Silva	IQSC-USP
10:50-11:10	Clustering Analysis Using Unsupervised Machine Learning with Clustering-Traj	Henrique M. Cezar	IF-USP
11:10-11:30	Understanding and Retaining the Perovskite Photo-active Phase for Solar Cell Applications	Srikanth Malladi	IQSC-USP
11:30-11:50	Fast Simulations of Ionic Liquids Confined by Metallic Planar Surfaces: Supercapacitors.	Matheus Giroto	IF-USP
12:00-14:00	<b>Lunch Time</b>		
14:00-14:20	A Combined Experimental and DFT investigation of Zero Dimensional Bismuth-Based Perovskites	Mailde da S. Ozório	IQSC-USP
14:20-14:40	Electronic Properties of Two-Dimensional Materials for Solar Energy Harvesting: Transition Metal Dichalcogenides of Fe-, Co-, Ni-, and Cu-Groups and their van der Waals Heterostructures	Rafael Besse	IFSC-USP
14:40-15:00	Data Mining and Statistical Tools based Framework to Investigate Quantum Chemistry Data	Johnatan Mucelini	IQSC-USP
15:00-15:20	<i>Ab initio</i> Study of the Adsorption Properties of $Au_4$ Clusters on $MoSe_2$ Nanoflakes	Naidel A. M. S. Caturello	IQSC-USP
15:20-15:40	Correlating Stability and the Properties of 55-Atom Bimetallic Pt-based Nanoalloys to Understand the Formation of Core-Shell Systems through Density Functional Theory	Paulo C. D. Mendes	IQSC-USP
15:40-16:00	<i>Ab Initio</i> Investigation of $CO_2$ Adsorption on $TM_{13}$ 4d Clusters	Krys Elly de A. Batista	UFPEL
16:00-18:30	<b>Posters + Coffee-Break – Project Discussions</b>		

**3rd Day – September 04, 2019** Chair: Lucas G. Verga

Location: IQSC – Anfi

Schedule	Description	Speaker
08:30-10:00	Molecular Dynamics Fundamentals: History, and Perspectives	Kaline Coutinho
10:00-10:30	<b>Coffee Break</b>	
10:30-11:15	Presentation of The LAMMPS Package: History, Use and Applications	Julian F. R. V. Silveira
11:15-12:00	Presentation of the GROMACS package: History, Use and Applications	Eudes Fileti

**4th Day – September 05, 2019** Chair: Augusto C. H. da Silva

Location: IQSC – Anfi

Schedule	Description	Speaker
08:30-10:00	Force Fields – First, Second, and Third Generation	Ricardo Paupitz B. dos Santos
10:00-10:30	<b>Coffee Break</b>	
10:30-12:00	Technical Details for Molecular Dynamics Calculations	André R. Muniz

**5th Day – September 06, 2019** Chair: Tuanan C. Lourenço

Location: IQSC – Anfi

Schedule	Description	Speaker
08:30-10:00	Most Important Properties in Molecular Dynamics Calculations	Luís Gustavo Dias
10:00-10:30	<b>Coffee Break</b>	
10:30-11:15	Introduction to <i>Ab initio</i> Molecular Dynamics	Diego Guedes-Sobrinho
11:15-12:00	Introduction to <i>Ab initio</i> Molecular Dynamics	Gustavo Troiano Feliciano

3rd Day – September 04, 2019

Location: IQSC – Sala B

3rd Day – September 04, 2019

Location: IQSC – Sala 100

CINE-CMSC Machine Learning Meeting  
08:00 – 12:00

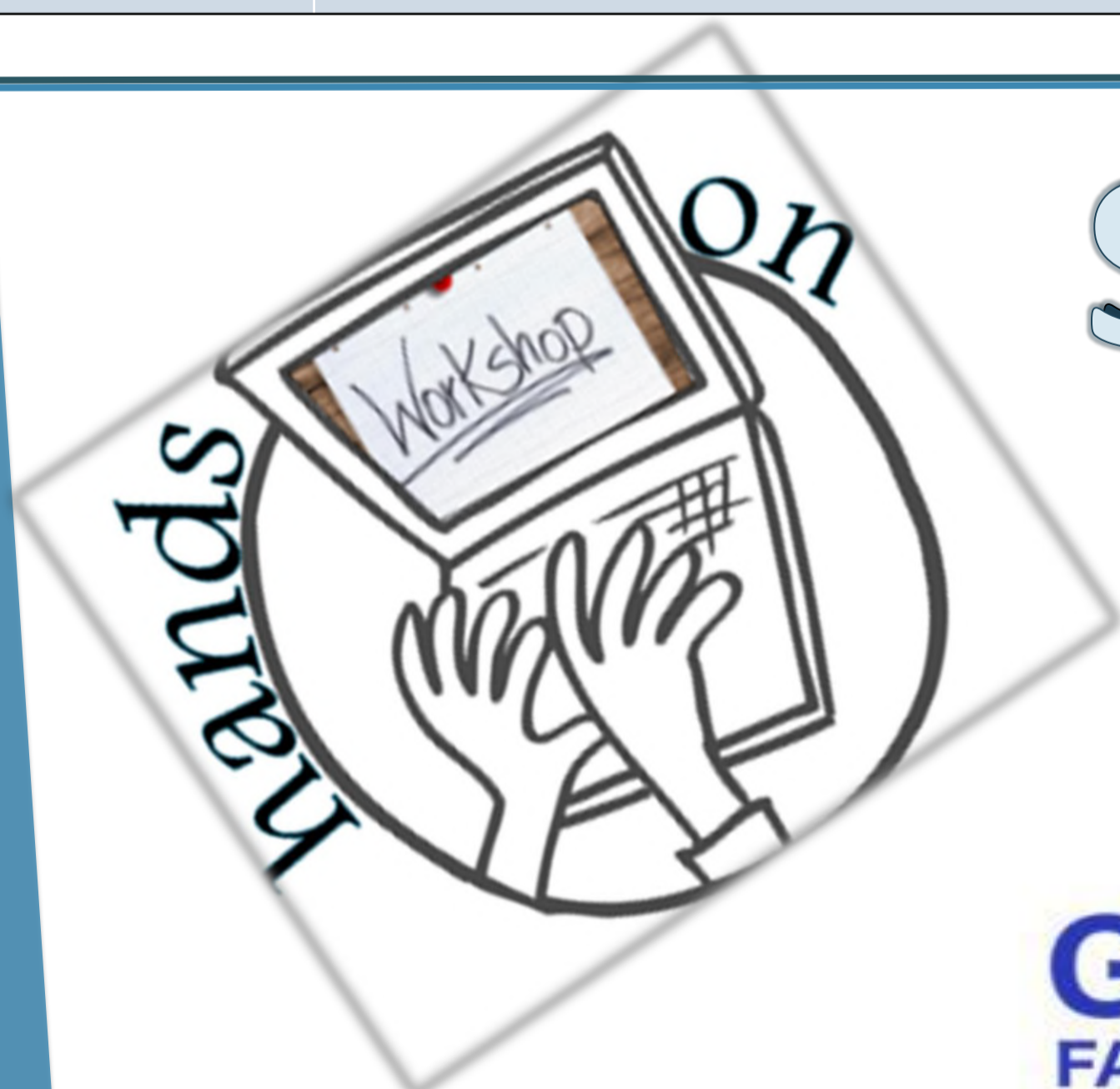
**Topics for Discussion**

- Scientific Integration.
- Papers in progress
- Expectations for the 18th month.

CINE-CMSC Project Evaluation 14:00 – 16:00

**Topics for Discussion**

- Scientific Integration.
- Collaborations within CINE.
- Challenge projects.
- FAPESP fellowships.
- Expectations for the 18th month.



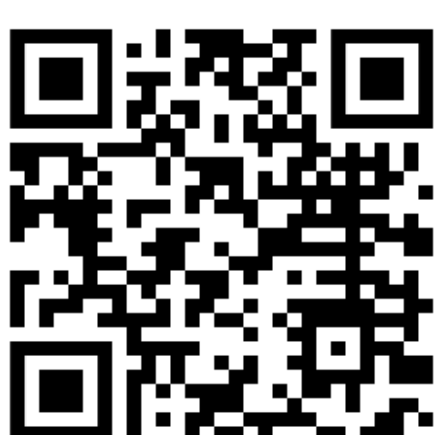
## September 4 – 6, 2019

### 14:00 - 18:00

**GROMACS**  
FAST. FLEXIBLE. FREE.  
Location: IQSC – Library



**LAMMPS**  
Location: IFSC – Laboratory 206



Live oral  
Presentations