



PÔLE OUEST

DU RÉSEAU FRANÇAIS DE CHIMIE THÉORIQUE

JOURNÉE SCIENTIFIQUE – 1 décembre 2020

De-Local Organiser

Institut des Matériaux Jean Rouxel, CNRS / Université de Nantes,
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If you do not have zoom installed yet, please visit <https://zoom.us/download>

Please set your name to include your institution in zoom, e.g. Chris Ewels (IMN Nantes)

Please turn off your microphone during the talks, you are very welcome to leave your camera on however! Equally we encourage you to take your coffee on-line for the possibility of group chats.

	09H20	<i>Bienvenue / Welcome</i>	
Chair 1	09H30	P1	Franck Tancret , IMN, Université de Nantes <i>Physics, chemistry and artificial intelligence for multi-objective combinatorial materials design: application to High Entropy Alloys</i>
	10H00	O1	Sergine Sarr , CEISAM, Université de Nantes, <i>Relativistic effects on the halogen bond in I-R-At</i>
	10H20	O2	Yuri Tanuma , IMN, Université de Nantes <i>Theoretical approach to carbon chain formation in carbon nanobelts</i>
	10H40	<i>- Pause-café / thé -</i>	
Chair 2	11H00	O3	Rudraditya Sarkar , CEISAM, Université de Nantes, <i>Multi-mode vibronic dynamics on small molecules and clusters</i>
	11H20	O4	Rabii Larhlimi , IC2MP, Université de Poitiers, <i>Computational Materials Discovery</i>
	11H40	O5	Ranim Mohamad , IMN, Université de Nantes, <i>Hydrogen embrittlement in nickel-based alloys</i>
	12H00	O6	Neha Tripathi , CEISAM, Université de Nantes, <i>Mechanism of action for Rad51 inhibitors via Molecular Mechanics</i>
	12H20	<i>- Pause Midi -</i>	

Chair 3	14H00	P2 Philippe Jund , CTMM, Université de Montpellier <i>Defects and their influence on the thermoelectric properties of materials : An ab-initio study</i>
	14H30	O7 William Lagargue-dit-Hauret , IMN, Université de Nantes, <i>Ab initio prediction of accessible oxidation states for transition metal impurities in semiconducting oxides</i>
	14H50	O8 Franck Gam , ISCR, Université de Rennes 1, <i>Electron counting in assemblies of three and more silver-rich superatoms</i>
	15H10	- Pause-café / thé -
Chair 4	15H40	O9 Ágota Tóth , INSERM-IPPRITT, Université de Limoges, <i>On the Interplay between Complex Lipid Bilayer Membrane and Multidrug Resistance-Associated Protein 1 (MRP1) by Means of Molecular Dynamics</i>
	16H00	O10 Hind Benzidi , INSA -GSM/Foton-IHM, Rennes <i>Materials properties for energy storage applications using first principle calculations</i>
	16H20	O11 Nina Tyminska , CTI, Université de Rennes 1, <i>Theoretical insights on electronic transport properties in a 2D Mn-benzo-quinoid frameworks</i>
	16H40	<i>News du pôle / du réseau</i>
	17H00	- Clôture -