



PÔLE OUEST

DU RÉSEAU FRANÇAIS DE CHIMIE THÉORIQUE

West pole SCIENTIFIC DAY -October, 25th 2021

Université de Rennes I, Amphi GrandJean, Bat 10B

Campus Beaulieu, Rennes

Plenary sessions (P) and oral communications (O) will last 45 and 20 minutes, respectively, including questions and/or comments.

	09H30	<i>Welcome breakfast</i>	
Chair 1	10H00	P1	George Volonakis , ISCR, Université de Rennes 1, <i>Ab initio computational material design and electronic structure of low-band gap perovskites</i>
	10H45	O1	Richail Dubien Mouladou-Koumba , IC2MP, Université de Poitiers, <i>Theoretical study of furfural derivatives reactivity/selectivity with alkynes: towards a potent valorisation route</i>
	11H05	O2	Mehdi Benmameri , IPPRIT, Université de Limoges, <i>Assessing membrane permeability of drugs using MD simulations</i>
	11H25	O3	David Vincent , ISCR, Université de Rennes 1, <i>Is BaCuF4 a high-temperature multiferroic material?</i>
	11H45	<i>- Lunch -</i>	
Chair 2	13H30	P2	Stéphane Téletchéa , UFIP, Université de Nantes, <i>COVID-19: past, present and future</i>
	14H15	O4	Théo Cavnac , IMN, Université de Nantes, <i>Modelling luminescence properties in solids: KCl and BaZrO3 as test cases</i>
	14H35	O5	Isabella Merritt , CEISAM, Université de Nantes, <i>Photoisomerisation quantum yields of Cis-Azobenzene: Dynamics on different excited state surfaces</i>
	14h55	<i>- Coffee/Tea break -</i>	
Chair 3	15H15	O6	Maxime Grasser , ISCR, Université de Rennes 1, <i>In silico CD & CPL spectra of lanthanide complexes</i>
	15H35	O7	Hamissou Mohaman , CEISAM, Université de Nantes, <i>Building a cost-effective methodology to study Ra(II) chemistry in solution</i>
	15H55	O8	Pooja Basera , FOTON, INSA Rennes, <i>Interfacial engineering to modulate surface dipoles, work functions and dielectric confinement of halide perovskites via surface passivation</i>
	16H15	<i>News from West Pole and ThéMoSiA National Federation</i>	
		<i>- Apéro & End -</i>	