



SESSION BL 1

TITLE	Theoretical insights in chemi- and bio-luminescence	
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ABSTRACT	<p>This session will aim to present the recent results on bio- and chemiluminescent systems obtained with theoretical tools. The systems involved in the chemiluminescent reactions are very challenging from the theoretical point of view as they imply excited states and states crossing. The modulation of light-emitted wavelengths can come from different molecules, protonation states or conformations, and from the influence of the environment. State of the art theoretical methodologies from quantum mechanics (QM), molecular mechanics (MM) and/or hybrid QM/MM are currently used to overcome the difficulties and solve the complex problems of chemi- and bio-luminescence. The session will deal with reactivity and/or spectroscopy of bio and/or chemiluminescent systems and will give opportunity to show to the experimentalists the potential of using theory to interpret experimental data and predict new mechanisms and how collaboration between theory and experiment can strength the research in this area.</p>	
KEYWORDS	Theory, computational modelling, reactivity, excited-state chemistry, spectroscopy	