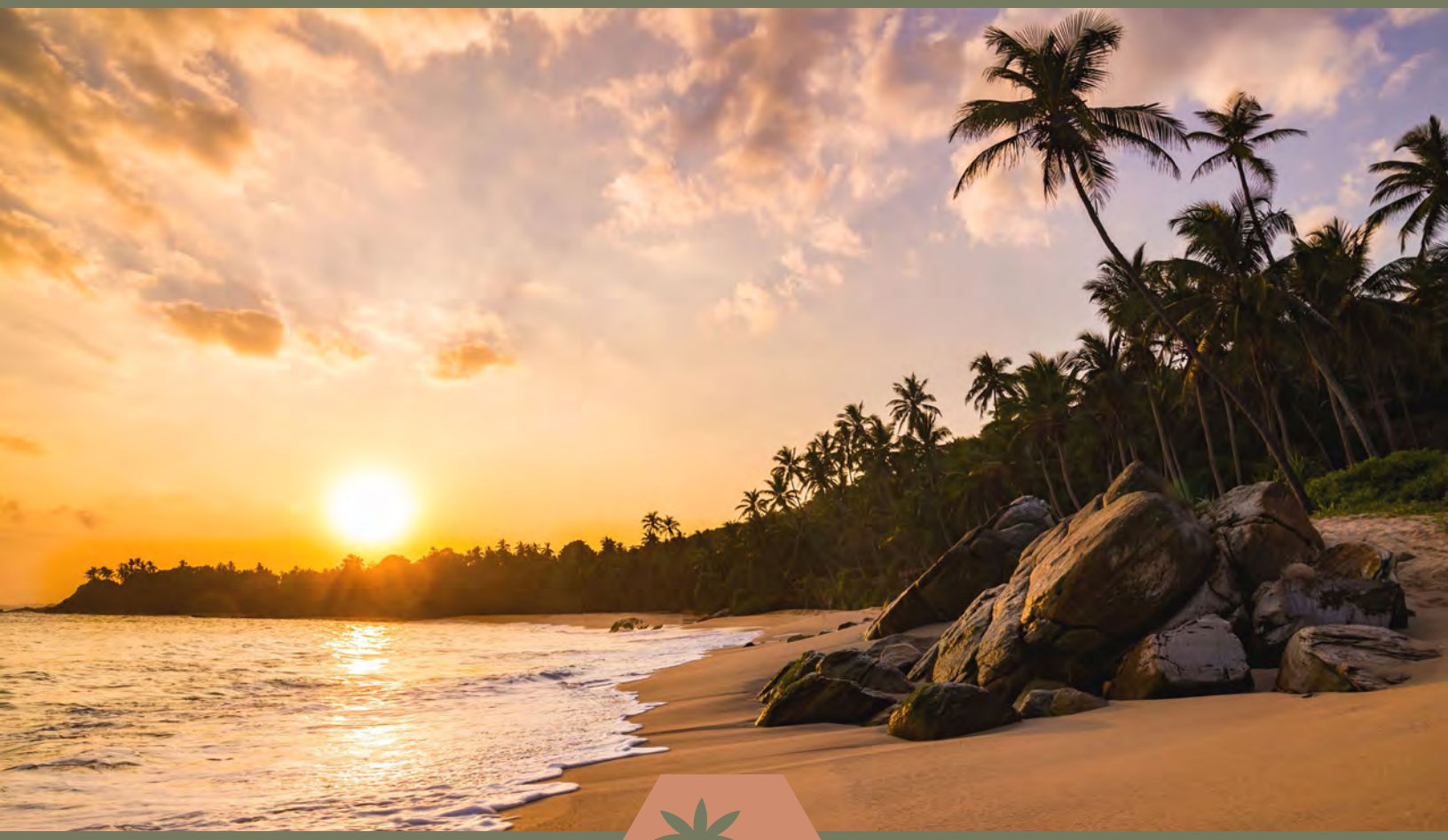
Program & Abstracts



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HALLOYSITE-BASED CATALYSTS: COMPUTATIONAL AND EXPERIMENTAL INVESTIGATIONS INTO BIOMASS CONVERSION

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Halloysite is a natural clay mineral with a hollow tubular structure, applicable as a component of biocompatible nanosystems with specific functionalities. Its particular morphology can be exploited to obtain various organic-inorganic composites that can be used for different types of applications such as nanoreactors for various types of chemical processes. In the last decades the selective oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDCA) has become one of the most important reactions that involves the use of biomass and its derivatives. FDCA is one of the most requested chemical compounds: it should in fact be used for the production of polyethylene furanoate, a bioplastic that could replace PET. This study involves the modification of halloysite nanotubes outer surface with an organosilanic compounds, like AEAPTMS. These modifications aim to facilitate the binding of gold nanoparticles on the nanotube surface. Subsequently, the modified nanotubes are explored as heterogeneous catalysts in the oxidation of HMF to FDCA. Both computational and experimental methods are employed to investigate the reaction pathway. The computational analysis focused on analyzing the first steps of the reaction with H_2O_2 as oxidizing agent and then going into a more in-depth analysis of the gold cluster growth. The experimental part consisted in the optimization of a synthesis strategy of the gold nanoparticles and then their linking to the beforehand modified halloysite surface as the starting catalyst for the biomass conversion.