

## Poster

**Enhanced Photostability and Efficacy of Hybrid Zeolite-Encapsulated UV Filters for Sunscreen Applications****R.Arletti<sup>1</sup>, R. Fantini<sup>1</sup>, M. Fischer<sup>2</sup>, R. Cavalli<sup>3</sup>, M. Argenziano<sup>3</sup> L. Mino<sup>4</sup>**<sup>1</sup>*Department of Chemical and Geological Sciences, University of Modena and Reggio Emilia, Modena, Italy*<sup>2</sup>*Crystallography & Geomaterials Research, Faculty of Geosciences, and Bremen Center for Computational Materials Science, and MAPEX Center for Materials and Processes, University of Bremen, Bremen, Germany*<sup>3</sup>*Dipartimento di Scienza e Tecnologia del Farmaco - Università degli Studi di Torino, Torino, Italy.*<sup>4</sup>*Department of Chemistry and NIS Centre, University of Torino, Torino, Italy)*[rossella.arletti@unimore.it](mailto:rossella.arletti@unimore.it)

Exposure to both UVA and UVB radiation from the sun stands as the primary cause of skin cancers. Sunscreen products have become ubiquitous in personal-care products, packaging, plastics, dyes, and many other sectors. Ideal UV filters should be photostable and dissipate the absorbed energy efficiently. However, most organic UV filters are photolabile upon protracted UV exposure, leading to the formation of photoproducts of unknown toxicity for human health and environment. The chemical environment surrounding UV filters may strongly affect their behaviour: the interaction with other components of sunscreen formulations may enhance their degradation. Therefore, much effort has been invested in developing more effective and safe sunscreens.

Our team recently focused on the preparation and characterization of hybrid UVfs obtained by the encapsulation of organic UV filters into various zeolites differing for topology [1,2]. The most efficient zeolites for the encapsulation of organic UV filters, in term of stability and efficiency in radiation filtration, resulted to be potassium LTL and sodium FAU zeolites. This work reports the results of combined crystallographic investigation carried out exploiting X-ray powder diffraction, Fourier-transform infrared spectroscopy, and density functional theory (DFT).

Regarding LTL/OMC ZEOfilter, IR data indicate a perturbation of the  $\nu(\text{C}=\text{O})$  mode of the OMC carbonyl group and this was confirmed by structural refinement, highlighting that the reason of stability was the bond between molecules and the extraframework K.

The combination of IR and DFT was crucial to identify all the complex host-guest interactions occurring inside the FAU/OMC hybrid and to unveil that, although slightly thermodynamically unfavored, OMC is dominantly present in the trans form inside the NaX framework. Even for this hybrid, the interaction molecule-cations is the key feature for its stability and efficacy.

In addition, in this work, we report further proof indicating that the use of this encapsulate filter could potentially substitute for conventional UVfs. In fact, the hybrids were successfully incorporated into oil-in-water emulsions and permeation tests displayed a very low UV filter permeation through no UV filter accumulation in dermis layer, moreover the photostability of the hybrid-based emulsions resulted to be higher with compared with that of bare filter emulsions

[1] Fantini et al. (2021) *Materials* 328 (2021) 11147.

[2] Confalonieri et . (2022) *Microporous and Mesoporous Materials*, 344, Article number 112212.