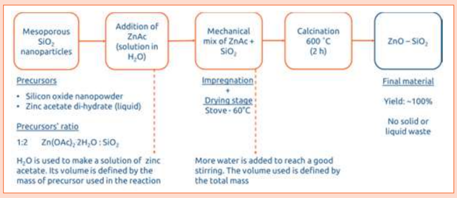
CIAC case study

March 2023

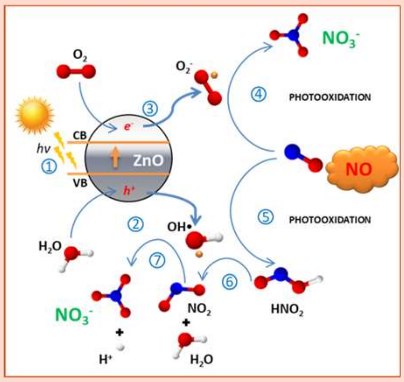
SiO_2-ZnO

SYNTHESIS FLOWCHART



MCNM USE

SiO_2-ZnO can be utilised in building coatings for photocatalytic NO_X decontamination. **ZnO** has photocatalytic properties and generates ROSs upon exposure to sunlight, water, and oxygen. NO_x gases are oxidised to nitrates; nitrates deposit on the surface after the conversion, and are cleared by rain. **SiO_2** improves ZnO performance, stability, compatibility, and dispersibility in the construction materials (e.g., mortar).



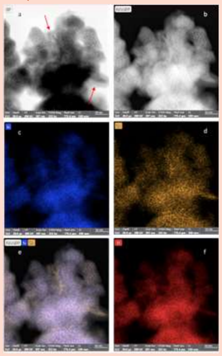
CHARACTERISATION

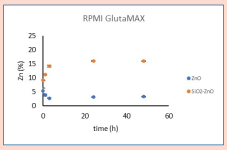
Extensive characterisation was carried out by partners at CNR-ISTEC, CSIC and UNIVE.

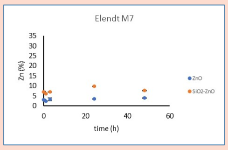
- Average primary particle size (nm) by TEM and shape: 17±3 nm; semi-spherical
- Specific surface area, pore volume and porosity:

	Specific surface area (m^2/g) by BET	Pore volume (cm^3/g) by BET	Porosity
SiO_2	119.2±0.6	0.170±0.008	mesoporous
SiO_2-ZnO	48.7±0.2	0.142±0.007	mesoporous

- Elemental composition by ICP-OES (%): 80% SiO_2; 20 ZnO% (small amount of Al, B, Fe, Na and Ti based impurities)
- Tests conducted with HR-TEM-EDX: signal of Si, Zn and O, suggesting that the SiO_2 NPs are covered by ZnO
- Preliminary dissolution experiments: in different ecotox and tox media, Zn(II) dissolution % from SiO_2-ZnO was always ~2 times higher than for ZnO, excepting for the PSF (pH: 4.5) → possibly due to different geometry of ZnO alone versus on SiO_2 particles



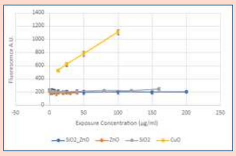


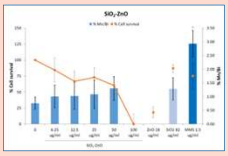


TESTING and SSbD MATERIAL

Human hazard testing

- SiO_2-ZnO shows no indication of oxidative stress (HWU) or inflammasome activation (RIVM)
- This MCNM indicates a dose-dependent cytotoxicity in three different types of testing (HWU, RIVM, SU); in all of them, SiO_2-ZnO was more cytotoxic than its corresponding concentration of ZnO alone



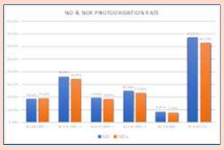


SSbD material

A new, SSbD version of SiO_2-ZnO (Tier2) was generated with liquid precursors, to reduce the occupational exposure during the production of the MCNM (CNR-ISTEC).

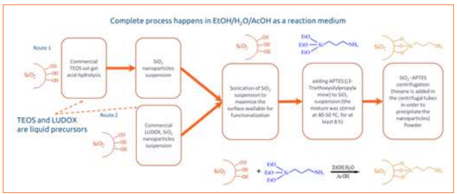
Photocatalytic testing

Pristine (Tier1) and SSbD (Tier2) SiO_2-ZnO were tested on their NO_X photooxidation rate ability at different percentages into the mortar (1-5%). Efficiency was similar for the 1% MCNM samples, but not for the 5% ones → improving the mortar-MCNM mixture and its composition might help increase the photocatalytic efficiency



SiO_2-APTES

SYNTHESIS FLOWCHART



MCNM USE

In building materials, nanoparticles can act as hydration nuclei, contributing to the development of cement hydration and to the enhancement of material properties (durability, mechanical, thermal, electrical performance and resistance to conductivity, etc.). However, the agglomeration occurring with nanoparticles compromises their ability to enhance material's properties. NP dispersion can, therefore, be improved through functionalisation.

SiO_2 can improve the mechanical resistance of building materials (+20% compressive strength compared to untreated concrete). Its functionalisation with **APTES**, a silane, improves SiO_2 dispersibility in concrete/mortar

SiO_2-APTES improves the mechanical performance of materials based on cement mortars and concrete:

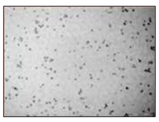
- Increases the rate of hydration
- Improves its compressive strength acting on the microstructure of the pastes - higher amount of CSH gel generated due to the pozzolanic relationship with $Ca(OH)_2$, reduction in porosity and therefore improvement in mechanical properties

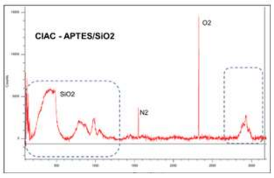
CHARACTERISATION

Extensive characterisation was carried out by partners at CNR-ISTEC, CSIC and UNIVE.

Characteristics	SiO2-APTES
Average primary particle size (nm) by TEM	20
Specific surface area (m2/g) by BET	104.7±0.7
Pore volume (cm3/g) by BET	0.58±0.03
Porosity	Mesoporous
Chemical identity by RAMAN	characteristic modes of silica and new modes, mainly at C-H region, have been identified
Chemical identity by DRIFTS after dehydration	the propyl chain of the APTES molecule have been determined but APTES molecules are not fully bonded either with the SiO2 surface or/and with themselves
Thermal stability by TGA	different behaviour among labs and among different batches within the same lab → maybe lack of homogeneity; further investigation is needed

- RAMAN spectroscopy: SiO_2-APTES analysed at 514 nm shows characteristic modes of silica and new modes, mainly at C-H region. Atmospheric N_2 and O_2 are also apparent at 1550 and 2324 cm^{-1} (CSIC)
- TEM imaging: obtained by CIAC

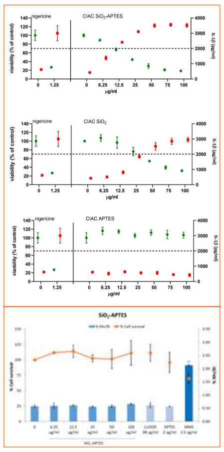




TESTING

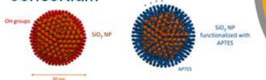
Human hazard testing

- SiO_2-APTES shows indication of inflammasome activation (RIVM): both MCNM and its SiO_2 component induce IL-1ß release, activating the inflammasome
- Two cytotoxicity methods conducted (WST-1 and RPD) to assess cell survival show differing results, as they look at different mechanisms of cell death in different cell types



MATERIAL MODELLING

A coarse-grained (CG) model of SiO_2-APTES NPs, with a diameter in the 10-20 nm range is being developed (UNIGE). The current work aims at the validation of the model, which will be based on the reproduction of (i) water contact angle on a flat SiO_2-APTES surface and on the reproduction of (ii) SiO2-APTES zeta potential, possibly measured within the SUNSHINE consortium



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