Smart leaching of essential oils from silica particles

Maialen Argaiz, Amaia M Goitandia, Miren Blanco, Estibaliz Aranzabe

[a] Química de Superficies y Nanotecnología , Tekniker, Eibar, 20600

e-mail: maialen.argaiz@tekniker.es

THE CONTEXT

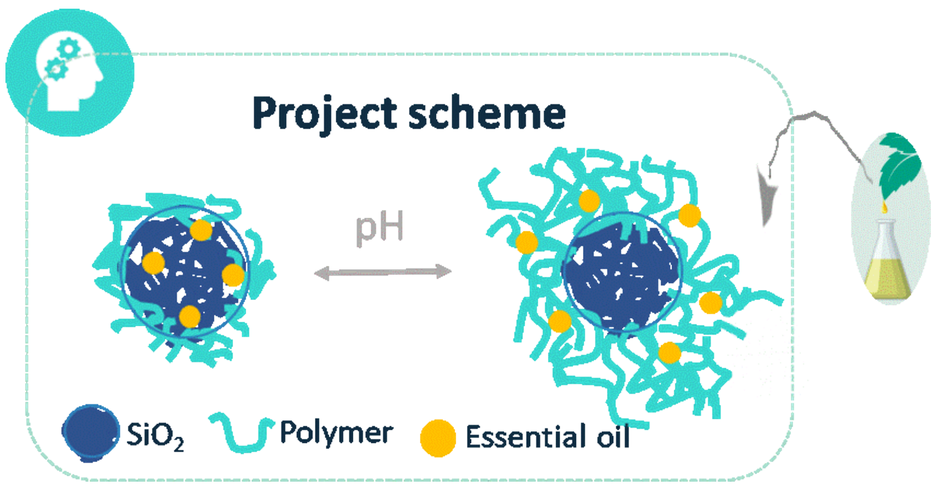
- Microbial colonisation of surfaces forms a **dangerous reservoir for pathogens** contributing to spread of infections which can cause significant cost in human life and economic terms.
- It is estimated that only **antimicrobial resistance infections are responsible for 110,000 deaths and EUR 1.5 billion per year in healthcare costs and productivity losses.**
- Several antimicrobial coatings exist in the market; however, they are **based mainly on the leaching of non-environmentally friendly chemicals** (i. e. non-biobased antimicrobial molecules such as antibiotics, phenolic biocides, or quaternary ammonium compounds) and are **formulated considering synthetic, non-biobased polymers as binders.**
- These antimicrobial coatings frequently show **serious concerns** linked to antibiotic resistance, complex chemical synthesis, environmental pollution, non-biodegradability, low product performance, toxicity and extremely low sustainability.
- Hence, there is a **real need of innovative high performance antimicrobial coatings** and also a significant market opportunity because the antimicrobial coatings market size exceeded USD 3.2 billion in 2019 and **is estimated to grow at over 10.4% CAGR between 2020 and 2026.**

RELIANCE

Addressing the growing need for an innovative holistic antimicrobial solution for different surfaces that is highly effective, safe and sustainable by design

The main objective of RELIANCE is to design and develop smart response **self-disinfectant antimicrobial nanocoatings** based on a new range of **antimicrobial copper doped mesoporous silica nanoparticles (Cu-SMIN) modified with non-toxic bioactives**, such as **essential oils (EOs) coming from non-edible plants**, incorporated into the porous particles for a **controlled release** to the environment.

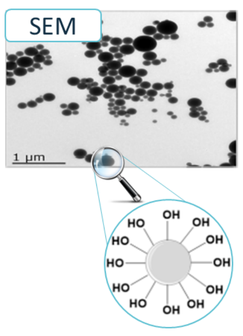
FUNCTIONALIZATION FOR SMART LEACHING



SiO_2 selection

nanografi

Commercial spherical (non-porous) **SiO_2** NP, APS: 0.3 µm



MONOMERS for functionalization

pH and T responsive monomers

2-(diethylamino)ethyl methacrylate) **DEAME** — pKa = 7.4

2-(dimethylamino)ethyl methacrylate) **DMAEMA** — pKa = 7-8

T responsive monomer

N-isopropylacrylamide **NIPAM**

0.03 and 0.06 mol/1.5 g SiO_2 NP

SYNTHESIS path

ATRP (Atom Transfer Radical Polymerization)

ATRP initiation process

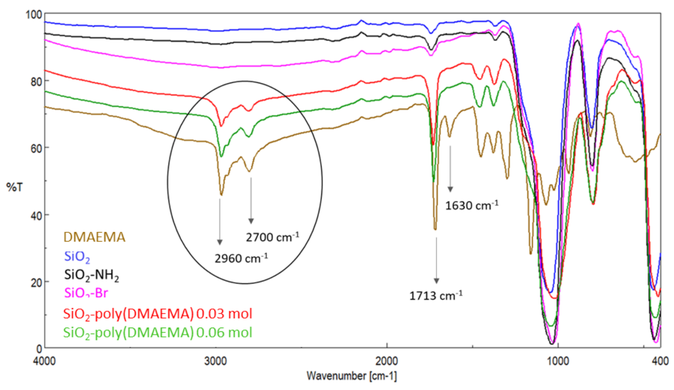
R-X (Initiator) + Mt/L (Activator, Lower oxidation state) ⇄ (Activation / Deactivation) R• (Active) + X-Mt+1/L (Deactivator, Higher oxidation state)

Main ATRP equilibrium

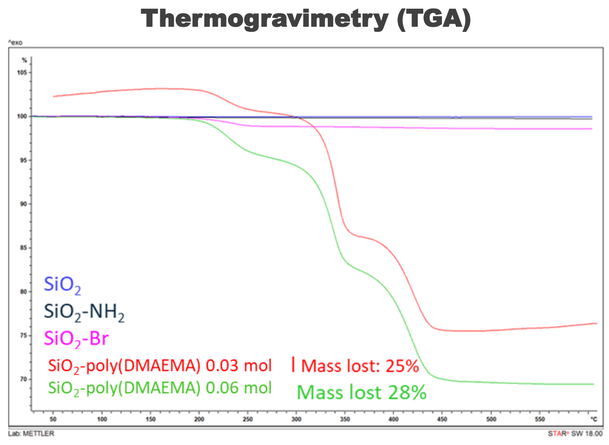
P_n-X (Polymer) + Mt/L ⇄ (Activation / Deactivation) P_n• (Active) + X-Mt+1/L

FUNCTIONALIZATION WITH poly(DMAEMA)

Fourier Transfer Infrared Spectroscopy (FTIR)



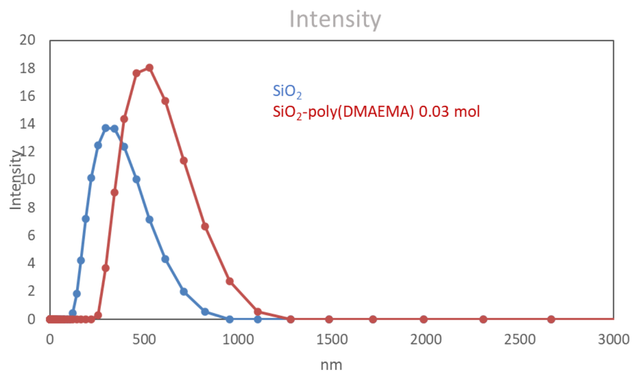
Thermogravimetry (TGA)



Absorption analysis (N quantification)

SiO_2	0.022 %N
SiO_2-NH_2 :	0.071 %N
SiO_2-Br :	0.031 %N
SiO_2-poly(DMAEMA) 0.03 mol:	3.09 %N
SiO_2-poly(DMAEMA) 0.06 mol:	3.39 %N

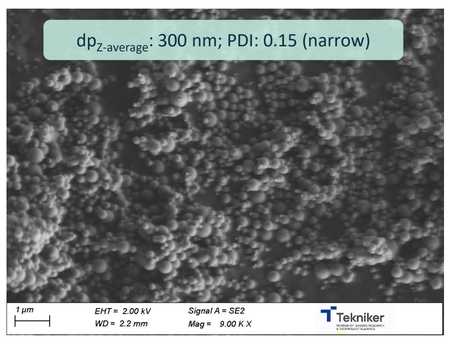
Dynamic Light Scattering (DLS)



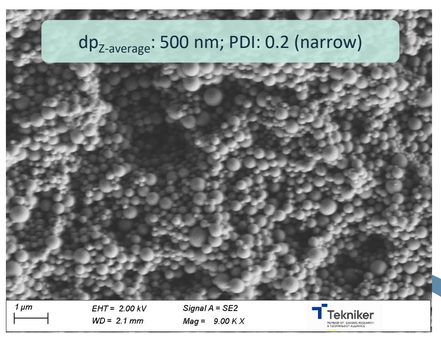
SMART RESPONSE to pH CHANGES

Scanning electron microscopy (SEM)

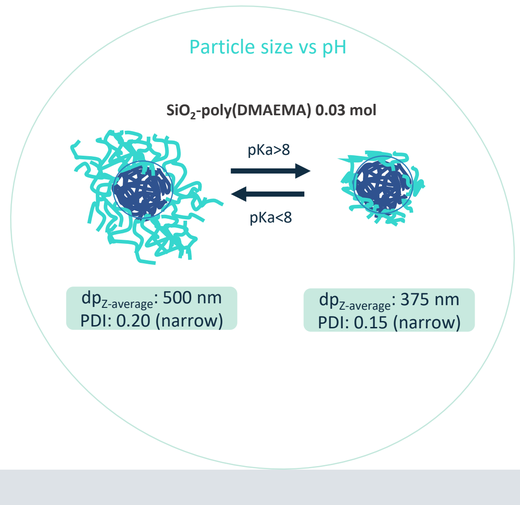
SiO_2



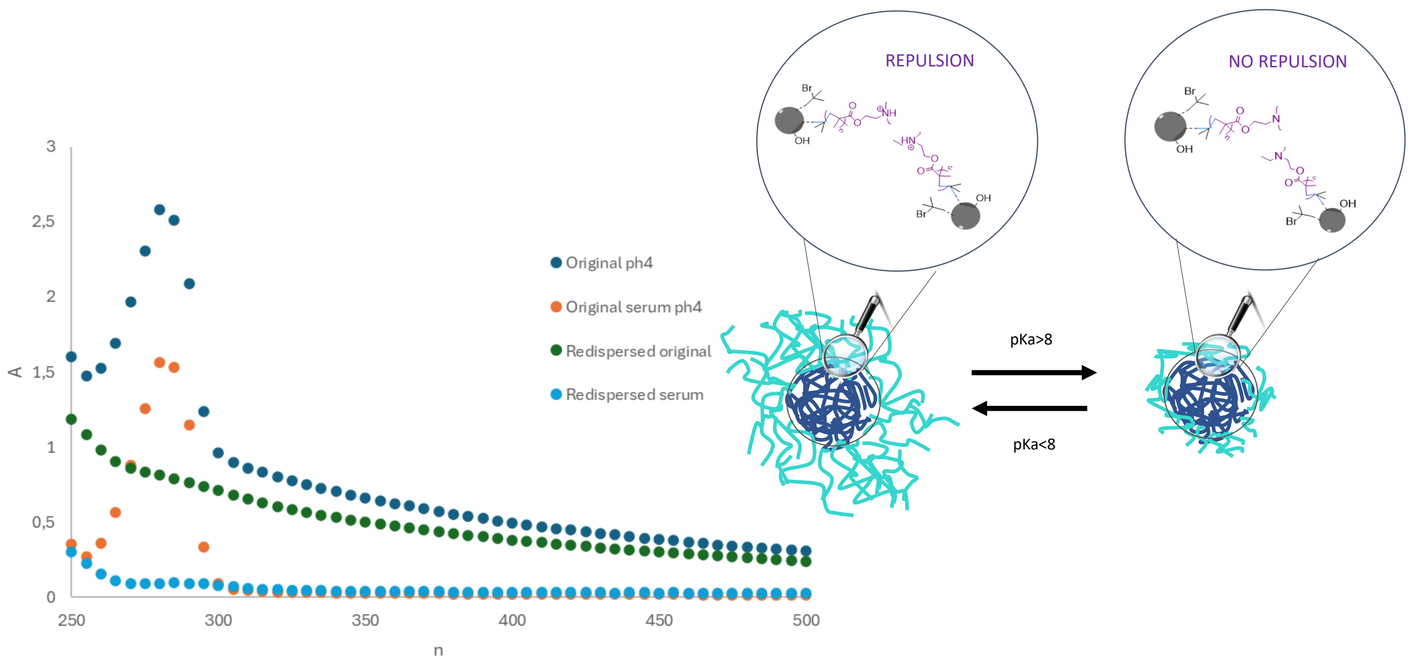
SiO_2poly(DMAEMA)



SMART RESPONSE



SMART RELEASE OF THE ESSENTIAL OIL



CONCLUSIONS

- **Efficient route for the synthesis of RESPONSIVE POLYMERS into SiO_2 NP**
- **The SiO_2 particles have been susccessfully functionalized → Assessed by FTIR, TGA, Elemental Analysis, SEM and DLS**
- **The polymeric brushes are responsive to pH changes → Assessed by DLS**
- **The release of the essential oils is not clearly observed. New evaluation routes are in-progress**

This project has received funding from the European Union's Horizon Europe Research and Innovation Programme under grant agreement No. 101058570 (RELIANCE). This output reflects only the author's view and the European Union cannot be held responsible for any use that may be made of the information contained therein