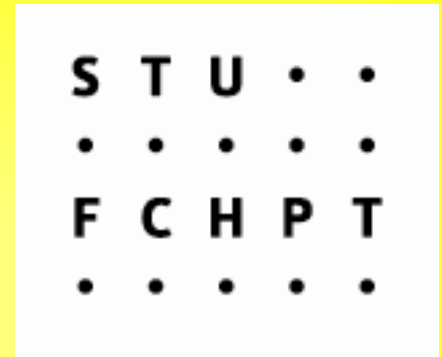


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## **Migration of nanoparticles from packaging and a sensor for the nanoparticles toxicity**



**Peter Šimon**

**COST Action FP1405 Meeting:  
Application and Communication of Active and Intelligent Packaging  
7-9 November 2017, Tzuba Hotel, Judean Hills, Israel**

# INTRODUCTION

**Nanomaterials** - applied worldwide

**Safety**, implications on human and environmental health and potential risks - under discussion

**Opinions** - from “completely harmless and safe” to “extremely hazardous”.

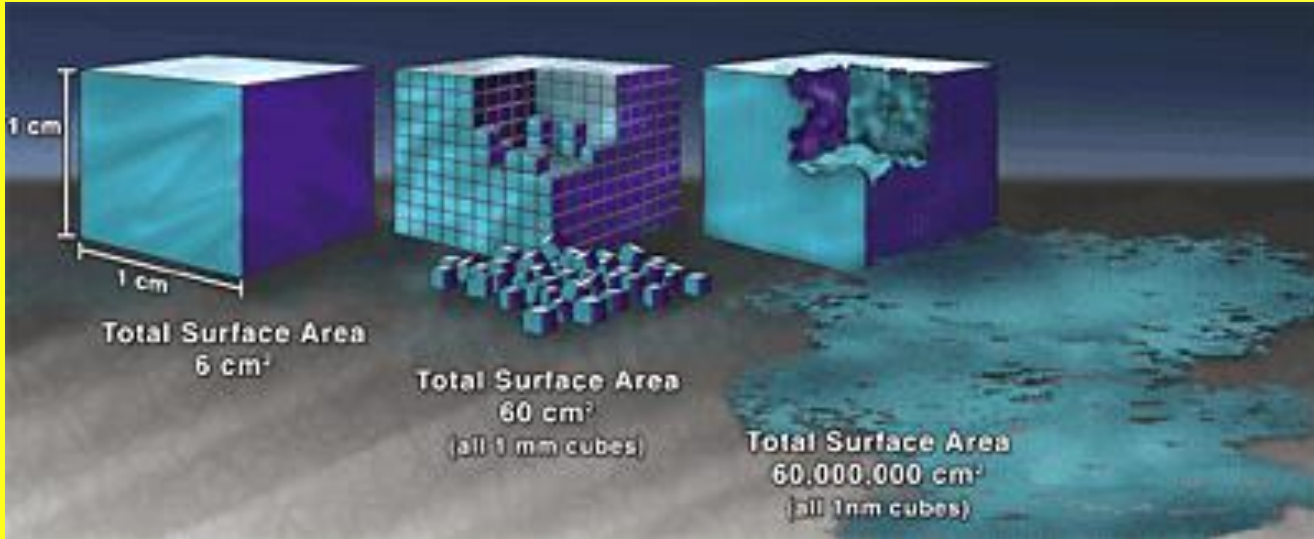
**Nanoscale** - having one or more dimensions of the order of 100 nm or less

**Size of pores in human body** - about 200 nm (gut), 70 nm (skin) ⇒ additional toxicity of NMs

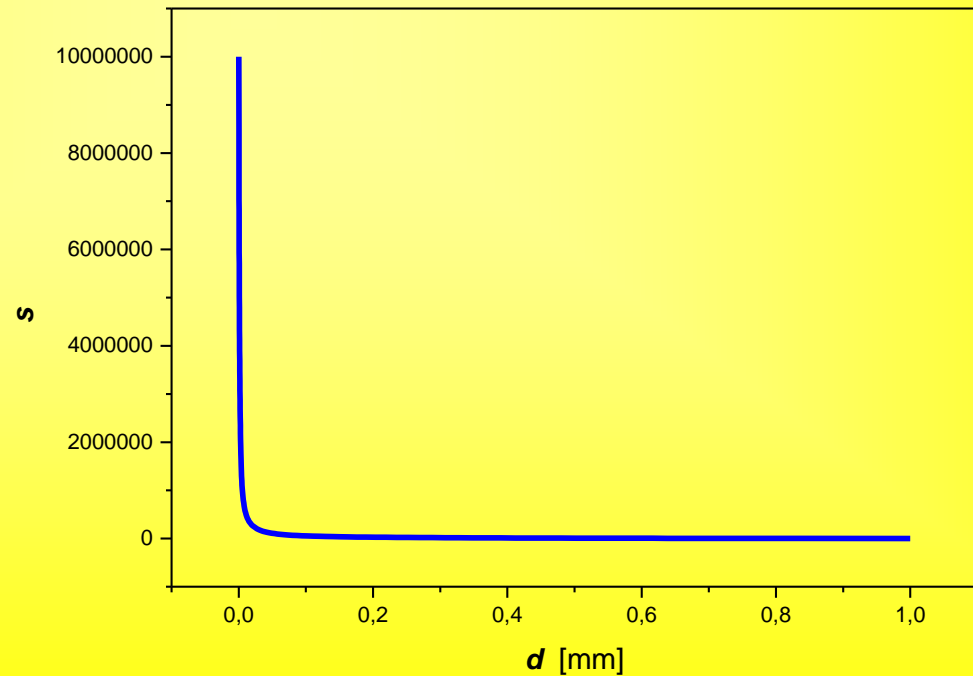
**Soluble and biodegradable NMs** – toxicity as the bulk counterparts

**Biopersistent NPs** – may accumulate

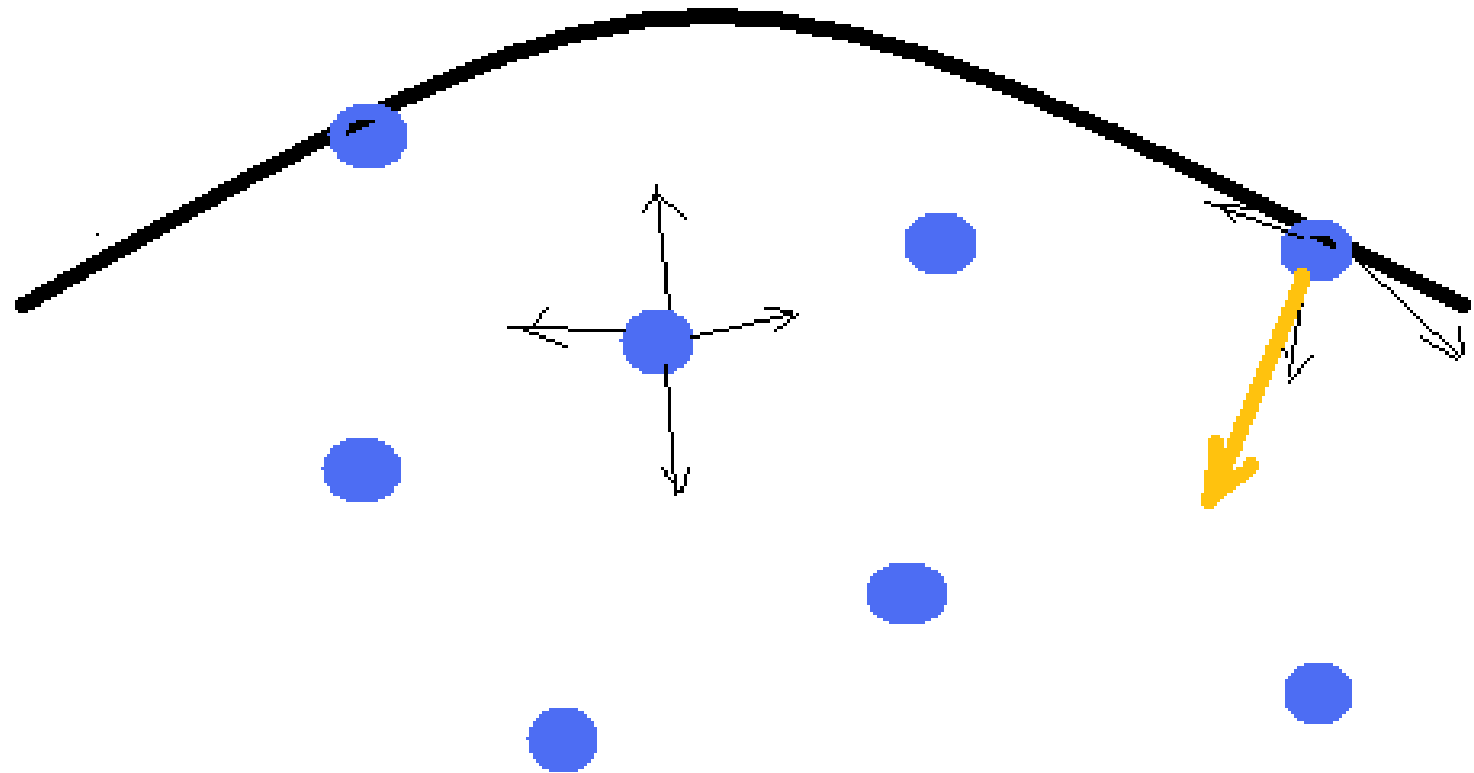
# Surface free energy and consequences



$$s = \frac{S}{V} \sim \frac{1}{d}$$



# Surface energy



Atoms/molecules on a solid surface miss the nearest neighbours above the surface - **unsatisfied bonds exposed to the surface.**

Surface atoms /molecules convey an extra potential energy = **surface free energy**

Due to the huge surface energy, NMs are **thermodynamically unstable** or metastable and exert **high chemical activity.**

**Properties of NPs differ from those of the bulk material**

# NANOPARTICLES IN FOOD

Biopersistent micro- and nanoparticles commonly found in food:

- silicon dioxide ( $\text{SiO}_2$ , E551),
- magnesium oxide ( $\text{MgO}$ , E530)
- titanium dioxide anatase ( $\text{TiO}_2$ , E171).
- The antimicrobial properties of nanosilver are known and such properties have recently been discovered for nano-zinc oxide and magnesium oxide

# NANOPARTICLES IN PACKAGING

- **filler – Ag, ZnO,  $\text{TiO}_2$ , etc. – intelligent packaging**
- **NPs from the matrix – toxicity not tested**

# Migration of nanoparticles from packaging to food

Stokes-Einstein relation:

$$D = \frac{k_B T}{6\pi\eta a}$$

The average distance,  $r$ , travelled by particles:

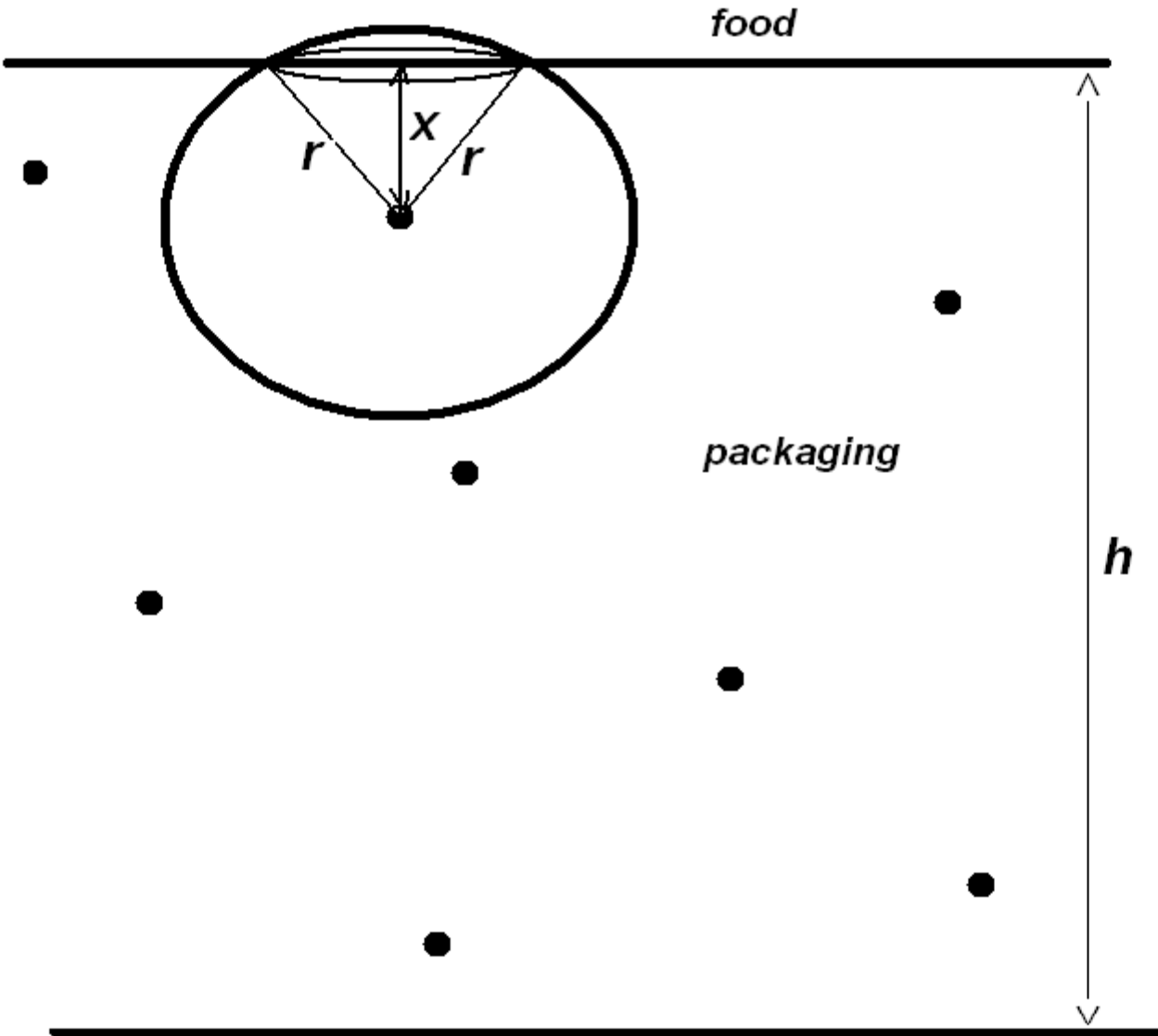
$$r = 2 \left( \frac{Dt}{\pi} \right)^{1/2} = \left( \frac{2k_B T t}{3\pi^2 \eta a} \right)^{1/2}$$

Williams-Landel-Ferry equation for polymer melts:

$$\eta(T) = \eta(T_g) \exp \left[ - \frac{C_1 (T - T_g)}{C_2 + T - T_g} \right]$$

The ability of NPs to migrate from the packaging to food, i.e. the migratability ( $m$ ):

$$m = \frac{n}{Sc_0} = \frac{1}{4} \left( \frac{2k_B T t}{3\pi^2 \eta a} \right)^{1/2} = \left( \frac{k_B T t}{24\pi^2 \eta a} \right)^{1/2}$$



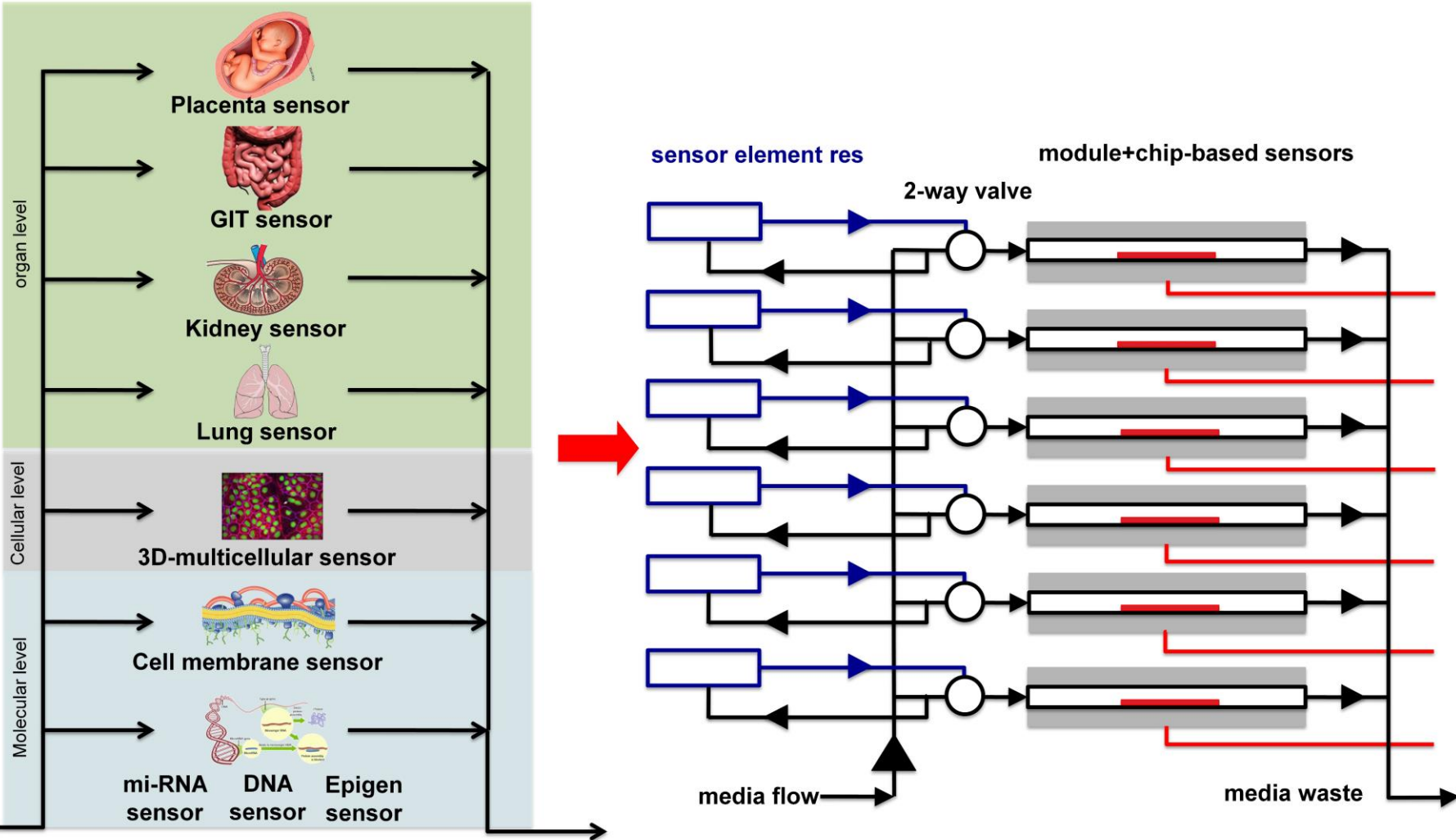


Polymer	<i>m</i> [m]	<i>m</i> [m]	<i>m</i> [m]	<i>m</i> [m]	<i>m</i> [m]	<i>m</i> [m]
	25 ° C	25 ° C	4 ° C	4 ° C	-18 ° C	-18 ° C
	1 month	1 year	1 month	1 year	1 month	1 year
LDPE	$3.7 \times 10^{-7}$	$1.3 \times 10^{-6}$	$2.5 \times 10^{-7}$	$8.9 \times 10^{-7}$	$1.9 \times 10^{-7}$	$6.7 \times 10^{-7}$
HDPE	$2.6 \times 10^{-7}$	$9.2 \times 10^{-7}$	$1.5 \times 10^{-7}$	$5.3 \times 10^{-7}$	$6.9 \times 10^{-8}$	$2.4 \times 10^{-7}$
PP	$1.5 \times 10^{-7}$	$5.2 \times 10^{-7}$	$5.1 \times 10^{-8}$	$1.8 \times 10^{-7}$	$8.0 \times 10^{-9}$	$2.8 \times 10^{-8}$
PET	$< 3.0 \times 10^{-9}$	$< 1.0 \times 10^{-8}$	$< 2.9 \times 10^{-9}$	$< 1.0 \times 10^{-8}$	$< 2.8 \times 10^{-9}$	$< 9.7 \times 10^{-9}$
PS	$< 2.1 \times 10^{-9}$	$< 7.4 \times 10^{-9}$	$< 2.0 \times 10^{-9}$	$< 7.1 \times 10^{-9}$	$< 2.0 \times 10^{-9}$	$< 6.8 \times 10^{-9}$

Migration of NPs from packaging to food will be detected mainly in the case of:

- very small NPs with the radius in the order of 1 nm
- from the polymer matrices that have a relatively low dynamic viscosity,
- from the polymer matrices that do not interact with the NPs.
- These conditions could be met for nanocomposites of silver with polyolefines (LDPE, HDPE, PP).
- For bigger NPs that are bound in polymer matrices with relatively high dynamic viscosity, the migration will not be detectable.
- This corresponds to nanosilver composites with PET and PS, and surface-modified montmorillonite embedded in various polymer matrices.

# Sensor platform for the NPs toxicity: Project H2020 HISENTS



**Toxicity** – depends on the concentration of NPs and contact time

**Physiologically Based Pharmacokinetic model**

**PBPK model** – a multicompartment model:

Description of :

**A**dsorption

**D**istribution

**M**etabolism

**E**xcretion

of chemical substances in an organism via a series of differential kinetic equations

**Parameters for the model – from the sensor platform -  
*Human on a chip***

# Conclusions

- 1. Nanomaterials** – may enter unusual sites in the body
- 2.** Biopersistent nanomaterials may accumulate
- 3.** Packaging – sources of NPs: filler, matrix
- 4.** Toxicity of nanomaterials – not fully clear in many cases
- 5. Sensor platform for NPs toxicity** – measuring the response of cells and modelling the response of mammals – *human on a chip*

## Acknowledgements:

- COST Action FP1405 **ActinPack**
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## Some publications:

1. Šimon P. & Joner E., *Journal of Food and Nutrition Research* **47** (2008) 51-59: Conceivable interactions of biopersistent nanoparticles with food matrix and living systems following from their physicochemical properties.
2. Šimon P., Chaudhry Q. & Bakoš D., *Journal of Food and Nutrition Research* **47** (2008) 105-113: Migration of engineered nanoparticles from polymer packaging to food – a physicochemical view.

A scenic sunset over a wide river. The sun is low on the horizon, creating a bright orange and yellow glow that reflects on the water's surface. A suspension bridge is visible on the left side of the river, and a silhouette of a church with a spire is on the right. The sky is filled with soft, wispy clouds.

**Thank you for  
your attention!**

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