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Cloé Desmet holds a PhD in Biochemistry, received from the University of Lyon in 2013 for her thesis on multiplex detection of biological markers and chemicals dedicated to diagnosis and environmental monitoring. She worked for the French Alternative Energies and Atomic Energy Commission (CEA, Grenoble) and the European Commission Joint Research Centre (EC-JRC, Ispra) where she completed her expertise in biosensors along the course of applicative projects for diagnostics, security and environmental monitoring. She also has experience in nanobiosciences, working on nanomaterial characterization and nano-based sensors.
In her current role at the JRC, she is involved in projects related to nanoplastics, nanoparticles characterization and sensor development for medical applications.

**"Characterization of nanomaterials hydrophobicity: from research to harmonized testing"**

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**Background, Motivation and Objective**
Several legislative frameworks, including the EU REACH Regulation 1907/2006, require reporting the octanol/water partitioning coefficient (Kow), an indicator of the fate and transport of a chemical in the aquatic compartment and a key parameter of any environmental exposure model. It has been demonstrated that nanoparticles cannot reach the thermodynamic equilibrium when partitioning between the octanol and water phases. For this reason, the use of Kow in nanomaterial risk assessment may lead to erroneous conclusions1. The OECD Working Party on Manufactured Nanomaterials concluded that the existing Test Guidelines for Kow determination are not applicable to (insoluble) nanoparticles and pointed out that a surrogate such as surface hydrophobicity may be necessary for obtaining information on nanomaterial environmental behaviour. In order to fill this technological gap, a new method for the quantification of nanoparticles hydrophobicity has been developed.

**Statement of Contribution/Methods**
The method is based on the quantification of the binding affinity of nanoparticles to rationally engineered hydrophobic and hydrophilic surfaces (collectors), via the analysis of their adsorption kinetics by Dark-Field microscopy2. Standard microscopy glass slides were coated first with a plasma deposited layer of polytetrafluoroethylene (hydrophobic) and then with

several layers of polyelectrolytes (PE) (poly(diallyldimethylammonium chloride), and polysodium 4-styrene sulphonate, to increase the hydrophilic character of the surface. The adhesion of PE layer thus permits the modification of the surface free energy components of the collectors3. Three collectors were produced and multi-channel liquid cells (Chipshop, Germany) were sealed on top. A conventional dark-field microscope (Leica DM-RME) was used for the measurement. Image sequences were recorded by a colour camera (Ace Basler) and the Trackmate plugin of ImageJ was used to detect and track single particles trajectories. The number of particles binding on the surface as a function of time could then be imported.

**Results/Discussion**

The surface energy potential acting between each couple nanoparticle-collector is calculated using the XDLVO theory, as the sum of the electrostatic potential, the Van der Waals potential and the hydrophobic potential4. The energy barrier (ΔGmax) induces the repulsion of the particles by the collector surface. The maximum binding rate is measured on a collector where ΔGmax = 0. When ΔGmax > 0, the particles binding rate on the collectors is reduced proportionally as follows: ΔGmax /kT = -ln v/vmax. Where v and vmax are the binding rates for the collectors with and without energy barrier respectively. ΔGmax depends on several known parameters (properties of the collectors and the particles) and some unknown parameters, including the polar component of the surface free energy of the particles (ΓP) that directly quantifies the hydrophobicity of the particles. Numerical solving routines were applied to extract the values for ΓP for all the studied particles. The measured ΓP values were also converted in a value of equivalent contact angle with water using the Owens-Wendt equation5.

The validity of the method was demonstrated with a robust set of particles with well-defined surface energy properties and exhibiting tuned hydrophobic character. An OECD Test Guideline based on this method, is under development and adoption is expected in 2021.

**1.** Praetorius et al., 2014, Environ Sci: Nano, 1, 317-323.
**2.**Valsesia et al., 2018, Commun Chem 1:53.
**3. Desmet et al., 2017, J Nanopart Res 19, 117.**
**4.** Donaldson et al., 2015, Langmuir 31 (7):2051-64.
**5.** Owens and Wendt, 1969, J Appl Polym Sci 13: 1741–1747.