



Advanced web tools for promoting the application of nanotechnology and the safe use of nanomaterials in the plastic sector

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Task Leader	ITENE			
Responsible Author	Name	Carlos Fito	E-mail	cfito@itene-com
	Beneficiary	ITENE	Phone	0034647521544

Rev. N°	Date	Author	Beneficiary name
1	28/10/2016	Sofia Ricarte	ITENE
2	13/01/2	Carlos Fito	ITENE

Participants		Contact
Packaging, Transport and logistics research center		Carlos Fito Email: cfito@itene.com
ProtoQSAR 2000 SL		Rafael Gozalbes rgozalbes@protoqsar.com
Universitat Rovira I Virgili		Alberto Fernandez alberto.fernandez@urv.cat
International Iberian Nanotechnology Laboratory		Begoña Espina Begona.Espina@inl.int
Centre National de la Recherche Scientifique		Virginie Serin serin@cemes.fr
Instituto Valenciano de Seguridad y Salud en el Trabajo		Esteban Santamaria santamaria_est@gva.es
Universidade do Porto		Riccardo Concu ric.concu@gmail.com

EXECUTIVE SUMMARY

The present document compiles information on the properties of the engineered nanomaterials selected in the project, including physical and chemical properties, toxicological and ecotoxicological data, as well data on the applications and uses of the ENMs selected in the project.

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1. General information on NanoDesk project

The members of the consortium designed a specification sheet based on the current needs of the industry, considering both regulatory issues and applications. The following table depicts the structure of the information sheets defined.

Identification of the substance	
Substance name	
EC	
CAS	
IUPAC	
Molecular formula	
Forms in the market	
Physical and chemical properties	
Shape	
Size (nm)	
Toxicological information	
Inhalation acute toxicity	
Dermal acute toxicity	
Oral acute toxicity	
Genotoxicity	
Citotoxicity	
Ecotoxicological information	
Freshwater Acute toxicity (Daphnia)	
Freshwater Acute toxicity (Alga)	
Freshwater Acute toxicity (Fish)	
Soil invertebrates (worms)	
BAF-Bioaccumulation	
Application	
Industrial uses	
Improved properties	
Polymeric matrix	
Recomendations, comments	

The information compiled into the information sheets have been also transferred to a Microsoft EXCEL spreadsheets, as well as an ACCESS database.

2. Available information sheets

2.1. Titanium Dioxide

Identification of the substance TiO₂

Substance name	Titanium dioxide
EC	236-675-5
CAS	13463-67-7
IUPAC	Titanium dioxide
Molecular formula	TiO ₂
Forms in the market	Powder; Nanorods, 1% aqueous solution; hydrophobized; Nanowires; aqueous suspension

Physical and chemical properties

Shape	Nanowires, nanotubes
Size (nm)	10, 20, 50-100, 4-8, 6

Toxicological information

Inhalation acute toxicity	Practically nontoxic
Dermal acute toxicity	No data
Oral acute toxicity	Nontoxic
Genotoxicity	Negative
Citotoxicity	Negative

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC ₅₀ = >100 mg/L (Nontoxic) EC ₅₀ = 42 mg/L (Practically nontoxic) EC ₅₀ = 29.8 mg/L (Practically nontoxic)
Freshwater Acute toxicity (Alga)	EC ₅₀ = 5.8 mg/L (Toxic) EC ₅₀ = 16.12 mg/L (Practically nontoxic)
Freshwater Acute toxicity (Fish)	LC ₅₀ = 124.5 mg/L (Nontoxic) LC ₅₀ = 20 mg/L (Tóxico)
Soil invertebrates (worms)	NOEC = >= 200 mg/kg soil dw
BAF-Bioaccumulation	No data

Application

Industrial uses	Plastic manufacturing Buildings and infrastructures Coatings
Improved properties	Dispersibility Gloss Durability UV Protection Drying
Polymeric matrix	Polyethylene (PE), polypropylene (PP), polystyrene (PS), polycarbonate (PC), polyamide (PA), polyvinyl chloride (PVC)
Recomendations, comments	Applied in high-temperature plastics applications Applied in interior and exterior coatings

2.2. Zinc Oxide

Identification of the substance: ZnO

Substance name	Zinc oxide
EC	215-222-5
CAS	1314-13-2
IUPAC	Zinc Oxide
Molecular formula	ZnO
Forms in the market	Dispersion in water (20%); Dispersion in ethanol (40%); Dispersion in butyl acetate (40%)

Physical and chemical properties

Shape	Spheric
Size (nm)	25

Toxicological information

Inhalation acute toxicity	LC50 = 1.79 mg/L (Very toxic)
Dermal acute toxicity	LD50 = >2000 mg/kg dw (Nontoxic)
	LD50 = > 5000 mg/kg bw
Oral acute toxicity	LD50 = > 333.33 mg/kg bw/day
	LD50 = > 5000 mg/kg bw
Genotoxicity	Negative
Citotoxicity	Negative

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	LC ₅₀ = 0.125 mg/L (Very toxic)
Freshwater Acute toxicity (Alga)	EC50 = 0.65 mg/L (Very toxic)
Freshwater Acute toxicity (Fish)	LC50 = 2 mg/L (Toxic)
	LC50 = 2.066 mg/L (Toxic)
Soil invertebrates (worms)	20 mg/L (Practically nontoxic)
BAF-Bioaccumulation	No data

Application

	Coatings
Industrial uses	Buildings and infrastructures
	Plastic
Improved properties	Long-term UV protection
Polymeric matrix	Polyvinylalcohol (PVA)
Recomendations, comments	For coatings, recommended for use in aqueous wood and furniture coatings for transparent systems

2.3. Silicon Dioxide

Identification of the substance: Silicon dioxide

Substance name	Silicon dioxide
EC	231-545-4
CAS	7631-86-9
IUPAC	Silicon dioxide
Molecular formula	SiO ₂
Forms in the market	Powder hydrophilic; Powder hydrophobic; aq. Suspension 30%; aq. suspension 50%; Pyrogenic (fumed) silica; Synthetic silica gels

Physical and chemical properties

Shape	Spherical
Size (nm)	10, 20

Toxicological information

Inhalation acute toxicity	Toxic
Dermal acute toxicity	Nontoxic
Oral acute toxicity	Nontoxic Practically nontoxic Toxic
Genotoxicity	Negative
Citotoxicity	Negative

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC50 = > 1000 µg/ml (Toxic) EC50 = 136.4 mg/L (Nontoxic)
Freshwater Acute toxicity (Alga)	EC50 = 10 mg/L (Practically nontoxic) EC50 = 388.1 mg/L (Nontoxic)
Freshwater Acute toxicity (Fish)	Toxic
Soil invertebrates (worms)	EC50 = 20 mg/L (Practically nontoxic)
BAF-Bioaccumulation	No data

Application

Industrial uses	Coatings / Plastic / Additives Viscosity reduction / Flow Mechanical properties/ Thermoplastic properties Nucleating agent out
Improved properties	Higher extrusion speeds / Flame retardant Abrasion resistance / Scratch resistance Reinforcement properties Rheological propoerties / Corrosion resistance Chemical resistance
Polymeric matrix	Acrylate copolymers, polyurethanes (PU), polyethylene terephthalate (PET) High temperature reactive diluent in aromatic and aliphatic epoxy resins Radiation-curing coatings. Recommended for solvent-free and solvent-borne radiation curable wood and furniture coatings as well as industrial coatings.
Recomendations, comments	PVC foams Rubber In additives, acts as a spacer agent

2.4. Cooper Oxide

Identification of the substance: Cooper oxide

Substance name	Cooper oxide
EC	215-269-1
CAS	1317-38-0
IUPAC	Cooper (II) oxide
Molecular formula	CuO
Forms in the market	No data

Physical and chemical properties

Shape	No data
Size (nm)	No data

Toxicological information

Inhalation acute toxicity	Very toxic
	Nontoxic
Dermal acute toxicity	No data
Oral acute toxicity	No data
Genotoxicity	No data
Citotoxicity	No data

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	LC50 = 2.6 mg/L (Toxic)
	LC50 = 1.7 mg/L (Toxic)
	LC50 = 2.6 mg/L (Toxic)
Freshwater Acute toxicity (Alga)	EC50 = 0.71 mg/L (Very toxic)
	EC50 = 0.8 mg/L (Very toxic)
Freshwater Acute toxicity (Fish)	DL50 = >100 mg/L (Nontoxic)
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Coatings
	Plastic
	Additives
Improved properties	Viscosity reduction
	Flow
	Mechanical properties
	Thermoplastic properties
	Nucleating agent out
	Higher extrusion speeds
	Flame retardant
Abrasion resistance	

2.5. Aluminum Oxide

Identification of the substance: Aluminum oxide

Substance name	Aluminum oxide
EC	215-691-6
CAS	1344-28-1
IUPAC	Aluminum oxide
Molecular formula	Al ₂ O ₃
Forms in the market	Powder

Physical and chemical properties

Shape	Spherical
Size (nm)	40 (average)

Toxicological information

Inhalation acute toxicity	LC50 = 0.888 mg/L (Extremely toxic)
Dermal acute toxicity	No data
Oral acute toxicity	LD50 = >1000 mg/kg (Nontoxic)
Genotoxicity	Negative ^{In vitro}
	Positive ^{In vivo}
Citotoxicity	Positive

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC50 = 310.53 mg/L (Nontoxic)
	LC50 = 53.29 mg/L (Practically nontoxic)
Freshwater Acute toxicity (Alga)	EC50 = 45.4 mg/L (Practically nontoxic)
	EC50 = 39.95 mg/L (Practically nontoxic)
Freshwater Acute toxicity (Fish)	No data
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Coatings
	Plastic automotive
Improved properties	Mechanical reinforcement
	Corrosion resistance
	Chemical resistance
	Scratch resistance
	Scuffing resistance
	Marring damage
	Rub-off damage
Polymeric matrix	Light scratching
	Transparency
	Acrylates (urethane acrylate, polyester acrylate, epoxy acrylate, polyether acrylate, acrylic acrylate) and aliphatic polyesters polyurethanes
	Solvent-free and solvent-borne, radiation-curable coatings and aqueous coating systems
Recomendations, comments	Polymer systems used in automotive and film application

2.6. Silver Nanoparticle

Identification of the substance: Nanoparticles of silver

Substance name	Nanoparticles of silver
EC	231-131-3
CAS	7440-22-4
IUPAC	Silver (1+)
Molecular formula	Ag
Forms in the market	Powder hydrophobic; powder hydrophilic, colloidal solution in water
Physical and chemical properties	
Shape	Triangular nanoprimis; Nanotubes; Compact
Size (nm)	1; 20; 35; 50; 100

Toxicological information

Inhalation acute toxicity	LC50 = 3.1x10 ⁶ particles/cm ³
Dermal acute toxicity	LD50 = >2000 mg/kg dw (Nontoxic)
Oral acute toxicity	LD50 = >2000 mg/kg dw (Nontoxic) LD50 = >5000 mg/kg dw (Nontoxic) Nontoxic
Genotoxicity	Nontoxic
Citotoxicity	No data

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC50 = 48.10 µg/L (Extremely toxic) EC50 = 0.187 mg/L (Very toxic) EC50 = 3844.1 µg/L (Toxic)
Freshwater Acute toxicity (Alga)	EC50 = 2.56 mg/L (Toxic) Toxic
Freshwater Acute toxicity (Fish)	LC50 = 9.4 mg/L (Toxic) LC50 = 250 mg/L
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Additives
Improved properties	Antibacterial properties Antimicrobial properties Thermal stability Power conversion efficiency
Polymeric matrix	Polyester (PS), polyethylene (PE), polyurethane (PU), polysulfone (PSU), nylon, silicone, polyimide (PI), polyether ether ketone (PEEK), polytetrafluoroethylene (PTFE), and polycarbonate (PC)

2.7. Layered Nanocalys

Identification of the substance: Nanoclays

Substance name	Nanoclays
EC	215-288-0
CAS	1318-93-0
IUPAC	Nanoclays
Molecular formula	(Na,Ca) _{0,3} (Al, Mg) ₂ Si ₄ O ₁₀
Forms in the market	Modified nanoclays, nanocrystals, platelets

Physical and chemical properties

Shape	No data
Size (nm)	No data

Toxicological information

Inhalation acute toxicity	No data
Dermal acute toxicity	No data
Oral acute toxicity	Nontoxic
Genotoxicity	Negative
Citotoxicity	Positive

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	NOEC = 100 mg/L (Nontoxic)
Freshwater Acute toxicity (Alga)	EC50 = 39.23 mg/L (Practically nontoxic)
Freshwater Acute toxicity (Fish)	NOEC = 100 mg/L (Nontoxic)
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Packaging Plastic Additives
Improved properties	Gas and moisture barrier Strength Toughness Abrasion resistance Chemical resistance Mechanical properties Thermal properties Structural properties Suitability for injection molding and extrusion Flame retardant Degree of dispersion Antimicrobial properties Tensile
Polymeric matrix	Polyamide (PA), polypropylene (PP), polyethylene terephthalate (PET), polyamides nylon, polyisobutylene (PIB), nylon nanoblends, poly(lactic acid) (PLA), epoxy, nitrile rubber (NBR), low density polyethylene (LDPE), EVA/PE compound, polyvinyl chloride (PVC)
Recommendations, comments	Incorporated in PET and used as additive for rubbers in combination with, for instance, TPO As additive in architectural coatings, mit to high PVC; and in other non-polymeric building materials As additive in elastomeric substrates and PET substrates

2.8. Carbon Black

Identification of the substance: Carbon black

Substance name	Carbon black
EC	215-609-9
CAS	1333-86-4
IUPAC	Carbon black
Molecular formula	Carbon black
Forms in the market	No data

Physical and chemical properties

Shape	No data
Size (nm)	No data

Toxicological information

Inhalation acute toxicity	Nontoxic
Dermal acute toxicity	No data
Oral acute toxicity	No data
Genotoxicity	Practically nontoxic
Citotoxicity	Practically nontoxic

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC50 = > 100 mg/L (Nontoxic)
Freshwater Acute toxicity (Alga)	EC50 = > 5mg/L (Toxic)
Freshwater Acute toxicity (Fish)	No data
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Ink and paints Additives
Improved properties	Strength Thermal properties UV Protection Electrical properties Antistatic Stability properties
Polymeric matrix	Polyacetylene (PA), poly(p-phenylene) (PPP), poly(p-phenylene vinylene) (PPV), poly(p-phenylene sulfide) (PPS), polyaniline (PANI), polypyrrole (PPy) and polythiophene (PT).
Recomendations, comments	Reinforcement effect in fillers is influenced by the interaction between the elastomer molecules, between the carbon black particles themselves, and between the carbon black particles and the elastomer matrix.

2.9. Graphene

Identification of the substance: Graphene

Substance name	Graphene
EC	231-955-3
CAS	7782-42-5
IUPAC	Graphene
Molecular formula	C
Forms in the market	Nanoplatelets, powder

Physical and chemical properties

Shape	Nanoplatelets, nanotubes
Size (nm)	3-6 (average)

Toxicological information

Inhalation acute toxicity	Toxic
	Toxic
Dermal acute toxicity	No data
Oral acute toxicity	Nontoxic
Genotoxicity	No data
Citotoxicity	No data

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	No data
Freshwater Acute toxicity (Alga)	No data
Freshwater Acute toxicity (Fish)	EC50 = 15.611 mg/L (Practically nontoxic) LC50 = 16.540 mg/L (Practically nontoxic)
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Packaging Additives
Improved properties	Mechanical properties Conductivity Tensile and yield strength Decrease gas permeability
Polymeric matrix	Polyethylene (PE), polypropylene (PP), polystyrene (PS), polycarbonate (PC), poly(methyl methacrylate) (PMMA), polyvinyl alcohol (PVA), poly(propylene carbonate) (PPC), polyvinyl chloride (PVC)
Recomendations, comments	Dispersion graphene in water

2.10. Fullerenes

Identification of the substance: Fullerenes

Substance name	Fullerenes
EC	No data
CAS	99685-96-8
IUPAC	Fullerenes
Molecular formula	C
Forms in the market	Powder

Physical and chemical properties

Shape	Spheric
Size (nm)	No data

Toxicological information

Inhalation acute toxicity	Nontoxic NOAEC: > 0.12 mg/m ³ (Nontoxic)
Dermal acute toxicity	Nontoxic
Oral acute toxicity	Nontoxic
Genotoxicity	Toxic
	Nontoxic
Citotoxicity	No data

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	Nontoxic Practically nontoxic
Freshwater Acute toxicity (Alga)	No data
Freshwater Acute toxicity (Fish)	LC50 = >350 mg/L (Nontoxic) Nontoxic
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Coatings
	Processability
	Dry speed
Improved properties	Electronic properties Antibacterial properties Friction resistance
Polymeric matrix	Polyketone (PK), polypropylene (PP), polyethylene (PE), nylon

2.11. Carbon Nanotubes – Singled Walled Nanotubes

Identification of the substance: Single Walled Nanotube

Substance name	Single Walled Nanotube
EC	231-153-3
CAS	308068-56-6
IUPAC	Single-Walled Carbon Nanotubes
Molecular formula	C
Forms in the market	Powder

Physical and chemical properties

Shape	Nanotube
Size (nm)	Diameter: 1,4 nm; Length: > 10 µm

Toxicological information

Inhalation acute toxicity	No data
Dermal acute toxicity	No data
Oral acute toxicity	LD50 = >50 mg/kg bw (Toxic)
Genotoxicity	Toxic
	Nontoxic
Citotoxicity	Negative

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC50 = >10 mg/L (Practically nontoxic) EC50 = 1.306 mg/L (Toxic)
Freshwater Acute toxicity (Alga)	EC50 = > 10mg/L (Practically nontoxic)
Freshwater Acute toxicity (Fish)	LC50 = > 10 mg/L (Practically nontoxic) LC50 = > 10 mg/L (Practically nontoxic)
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Plastic Additives
Improved properties	Toughness Mechanical properties Bonding strength Tensile strength Elastic modul
Polymeric matrix	Polymethyl methacrylate (PMMA), polypropylene (PP), thermoplastic polyurethane (PU), polyamide 66, polyamide 12, high density polyethylene (HDPE), low density polyethylene (LDPE), ethylene vinyl acetate (EVA), acrylonitrile butadiene styrene (ABS), polycarbonate (PC), fluorocarbons, nitrile rubber, poly(vinyl alcohol) (PVA), chitosan, polyimide (PI), polystyrene (PS), polyacrylonitrile polyaniline (PANI)
Recomendations, comments	Strengthened epoxy prepreg for numerous composites applications. Use molecular dispersion technology to ensure enhancements are evenly distributed throughout the resin

2.12. Carbon Nanotube – Multi Walled Nanotubes

Identification of the substance: **Multi Walled Nanotube**

Substance name	Multi Walled Nanotube
EC	936-414-1
CAS	308068-56-6
IUPAC	Multi-Walled Carbon Nanotubes
Molecular formula	C
Forms in the market	Charged, water soluble; not charged, hydrophilic powder

Physical and chemical properties

Shape	Tubes
Size (nm)	Diameter: 2-6 nm; Length: 1-10 μm

Toxicological information

Inhalation acute toxicity	EC50 = 2 mg/kg (Toxic) LC50 = 1.33 mg/m ³ (Toxic)
Dermal acute toxicity	LD50 = > 2000 mg/kg bw (Nontoxic)
Oral acute toxicity	LD50 = > 5000 mg/kg bw (Nontoxic)
Genotoxicity	Negative
Citotoxicity	Negative

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC50 = > 100 mg/L (Nontoxic)
Freshwater Acute toxicity (Alga)	EC50 = 134 mg/L (Nontoxic) EC50 = 120 mg/L (Nontoxic)
Freshwater Acute toxicity (Fish)	LC50 = >100 mg/L (Nontoxic)
Soil invertebrates (worms)	EC50 = >500 $\mu\text{g/L}$ (Very toxic)
BAF-Bioaccumulation	No data

Application

Industrial uses	Plastic Additives
Improved properties	Electrical conductivity Thermal conductivity Abrasion resistance Flame retardant properties Mechanical properties Antistatic behaviour Shielding against electromagnetic waves
Polymeric matrix	Fluorocarbons, polystyrene (PS), poly(9-vinyl carbazole) (PVK), polyacrylonitrile (PAN), polycarbonate (PC)

2.13. Gold Nanoparticles

Identification of the substance: Nanoparticles of gold

Substance name	Gold
EC	No data
CAS	7440-57-5
IUPAC	No data
Molecular formula	Au
Forms in the market	No data

Physical and chemical properties

Shape	No data
Size (nm)	No data

Toxicological information

Inhalation acute toxicity	No data
Dermal acute toxicity	No data
Oral acute toxicity	Toxic
Genotoxicity	No data
Citotoxicity	Negative

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC50 = >750 mg/L (Nontoxic) EC50 = >100 µm/L (Very toxic)
Freshwater Acute toxicity (Alga)	No data
Freshwater Acute toxicity (Fish)	EC50 = >100 µm/L (Very toxic)
Soil invertebrates (worms)	No data
BAF-Bioaccumulation	No data

Application

Industrial uses	Additives
Improved properties	Electrical conductivity
Polymeric matrix	Polyaniline (PANI), polystyrene sulfonate (PSS), polystyrene (PS), poly(dimethylsiloxane) (PDMS)

2.14. Calcium Carbonate

Identification of the substance: Calcium carbonate

Substance name	Calcium carbonate
EC	207-439-9
CAS	471-34-1
IUPAC	Calcium carbonate
Molecular formula	CH ₂ O ₃ Ca
Forms in the market	Powder

Physical and chemical properties

Shape	Cubic
Size (nm)	80 nm (average)

Toxicological information

Inhalation acute toxicity	No data
Dermal acute toxicity	LD50 = > 2000 mg/kg bw (Nontoxic)
Oral acute toxicity	NOAEL = 1000 mg/kg bw (Non toxic)
Genotoxicity	Negative
Citotoxicity	Negative

Ecotoxicological information

Freshwater Acute toxicity (Daphnia)	EC50 = > 1000 mg/l (Non toxic) LC50 = 159 mg/l (Practically nontoxic)
Freshwater Acute toxicity (Alga)	EC50 = > 100 mg/l (Practically nontoxic) EC50 = > 14 mg/l (Tóxico)
Freshwater Acute toxicity (Fish)	LC50 = > 100% v/v (Non toxic)
Soil invertebrates (worms)	EC50 value >> 0,07 g/ml (Non toxic)
BAF-Bioaccumulation	No data

Application

Industrial uses	Plastic Additives
Improved properties	Rheological properties Tensile properties Lower costs Strength Thermal properties Hardness
Polymeric matrix	Polyethylene (PE), polypropylene (PP), polyethylene terephthalate (PET), poly(lactic acid) (PLA)

3. Other Relevant Issues

More information on the characteristics of the nanomaterials will be available in the observatory of the safety of nanostructured polymers, as well as on the project web site, where updated EXCEL files will be available.