

Supplementary Materials: NanoDefiner e-Tool Knowledge Base Attributes

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Measurement technique (MT) recommendation for a specific material uses attributes, representing structured and formalized knowledge. For particle type description attributes listed in Table S1 are used to describe its physicochemical properties. Likewise, an MT is described via attributes listed in Table S2 (material-related properties), Table S3 (performance-related properties), and Table S4 (technical and economic properties). For MT recommendation not all MT attributes are matched.

Table S1. Matchable attributes for particle type description.

Attribute Name	Attribute description	Matched
trade_form	Trade form of particle type	Yes
dispersibility	Dispersibility of particle type by protocols	Yes
chemical_composition	Chemical compositions of particle type	Yes
composites	Composites of particle type	Yes
dimensions	Particle small dimensions number of particle type	Yes
shape	Particle shapes of particle type	Yes
analysis_temperature	Stable analysis temperature range of particle type (°C)	Yes
electron_beam	Particle type degradation under electron beam radiation	Yes
polydispersity	Grade of polydispersity in particle type	Yes
multimodality	Grade of multimodality in particle type	Yes
conductivity	Conductive properties of particle type	Yes
magnetism	Magnetic properties of particle type	Yes
functionalisation	Functionalisation of particle type	Yes
light_absorption	Light absorbing properties of particle type	Yes
fluorescence	Fluorescent properties of particle type	Yes
aggregation	Particle aggregation in particle type	Yes
agglomeration	Particle agglomeration in particle type	Yes
release_iam	Release of ions, atoms, and molecules of particle type	Yes
wr_size_range	Particle size range (nm) in particle type	Yes
presence	Presence of different sized subnano (diameter < 1 nm in all dimensions) or susnano (diameter > 100 nm in all dimensions) particles in particle type	Yes
os_vacuum	Degradation of particle type under vacuum	Yes

Table S2. Matchable material-related attributes for measurement technique description.

Attribute Name	Attribute description	Matched
trade_form	Material trade forms supported by MT	Yes
preparation	Suitable SOP-based preparation techniques for MT	No ^a
dispersion_medium	Dispersion media supported by MT	No ^a
dispersibility	Dispersibilities by protocols supported by MT	Yes
chemical_composition	Chemical compositions supported by MT	Yes
composites	Composites supported by MT	Yes
dimensions	Number of small dimensions supported by MT	Yes
shape	Particle shapes supported by MT	Yes
analysis_temperature	Analysis temperature range (celsius) of MT	Yes
electron_beam	Use of electron beam by MT	Yes
polydispersity	Grades of polydispersity supported by MT	Yes
multimodality	Grades of multimodality supported by MT	Yes
conductivity	Conductive properties supported by MT	Yes
magnetism	Magnetic properties supported by MT	Yes
functionalisation	Functionalization supported by MT	Yes
light_absorption	Light absorption supported by MT	Yes
fluorescence	Fluorescence supported by MT	Yes
aggregation	Aggregation supported by MT	Yes
agglomeration	Agglomeration supported by MT	Yes
release_iam	Release of ions, atoms, and molecules supported by MT	Yes

^a Not matched for MT recommendation, but takes effect on parts of the categorization workflow.

Table S3. Matchable performance criteria-related attributes for measurement technique description.

Attribute name	Attribute description	Matched
tier	Screening (tier 1) or confirmatory (tier 2) MT	No ^a
purpose	MT usable for specific purpose(s)/regulations	No ^a
disclaimer	MT disclaimer and important information for use	No ^a
multiconstituent	MT supports multi-type samples	No ^a
specific_technique	MT provides specific techniques	No
wr_size_range	Particle size range (nm) measured properly by MT	Yes
wr_concentration_range_type	Concentration range type specified by attribute wr_concentration_range	No
wr_concentration_range	Interpretation is dependent on attribute wr_concentration_range_type	No
wr_minimum_sample_type	Sample type specified by attribute wr_minimum_sample_type	No
wr_minimum_sample	Interpretation is dependent on attribute wr_minimum_sample_type	No
wr_linear_proportional_size	MT's results linear/proportional with respect to particle size	No
wr_linear_proportional_concentration	MT's results linear/proportional with respect to particle concentration	No
wr_detection_quantification_limit	Size range limits (nm-scaled) of particles MT measures properly	No
wr_sensitivity	Trust/usability/quality level regarding MT sensitivity	No
trueness	Trust/use/quality level regarding MT trueness	No
weighting_trueness	Trust/use/quality level regarding MT trueness in weighting size fractions	No
robustness	Trust/use/quality level regarding MT robustness	No
precision_type	Precision range type specified by attribute precision	No
precision	MT precision (nm-scaled)	No
resolution_type	Resolution range type specified by attribute resolution	No
resolution	MT resolution (nm-scaled)	No
size_distribution	MT supports measurement of size distribution	No
presence	MT supports presence of different sized subnano ($d < 1$ nm in all dimensions) or susnano ($d > 100$ nm in all dimensions) particles	Yes
sl_discr_nnp_same	MT supports the discrimination from non-nanoparticles of the same composition	No
sl_discr_nnp_same_robustness	MT provides robustness against different types of impurities in case of discrimination from non-nanoparticles of the same composition	No
sl_discr_nnp_diff	MT supports discrimination from non-nanoparticles of another composition	No
sl_discr_nnp_diff_robustness	MT provides robustness against different types of impurities in case of discrimination from non-nanoparticles of another composition	No
sl_discr_np_diff	MT supports discrimination from nanoparticles of another composition	No
sl_discr_np_diff_robustness	MT provides robustness against different types of impurities in case of discrimination from nanoparticles of another composition	No
measurement_aggr	MT supports particle measurement within aggregates	No
measurement_aggl	MT supports particle measurement within agglomerates	No
measurement_individual_particle	MT supports single particle measurement in size and number	No
constituent_particle_counting_aggr	MT supports particle measurement in aggregates	No
constituent_particle_counting_aggl	MT supports particle measurement in agglomerates	No
composition	MT provides information on the chemical composition	No
size_type	MT measurands (equivalent diameters, nm-scaled)	No
data_format	Analysis file data formats provided by the MT	No ^a
destructive	Sample destruction caused by the MT	No
os_vacuum	Demand of vacuum by the MT	Yes
os_sample_support	MT demands preparation of suited supports	No

^a Not matched for MT recommendation, but takes effect on parts of the categorization workflow.

Table S4. Matchable technical and economic attributes for measurement technique description.

Attribute	Description	Matched
direct_counting	MT support of yielding directly number-weighted size distribution	No
convertibility	MT conversion algorithm's quality	No
full_size_range	MT support of accessing the full size range according to EC NM definition	No
upper_size	MT approximate upper size limit	No
lower_size	MT approximate lower size limit (close to 1 nm)	No
smallest_particle_dimension	MT support of accessing smallest particle dimension	No
primary_particle_access_aggr	MT support of accessing primary particles within aggregates	No
primary_particle_access_aggl	MT support of accessing primary particles within agglomerates	No
availability	MT availability and wide use	No
standard	MT is a standard	No
reference	MT potential as reference method	No
eot_preparation	MT sample preparation time	No
eot_measurement	MT measurement time	No
eot_reduction	MT data reduction time	No
eot_total	MT total time until results	No
cost_instrument	MT instrument costs	No
cost_analysis	MT analysis costs	No
cost_efficiency	MT cost efficiency	No
expertise	MT required expertise	No
hyphenation	MT ability to be hyphenated to other methods.	No
vacuum	MT demand for vacuum intensity	No
sample_support	MT demand for preparation on suited supports	No
degradation	MT risk of chemical sample degradation during measurement	No