PARC roadmap for nanomaterials – exploring how PARC can contribute most usefully

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1. Introduction

The Partnership for the Assessment of Risks of Chemicals (PARC) is an interdisciplinary effort to develop next-generation chemical risk assessment approaches to protect human health and the environment [1]. It supports the European Union's Chemicals Strategy for Sustainability and the European Green Deal's "Zero pollution" ambition with new data, knowledge, methods, tools, expertise and networks.

Building on a previous human biomonitoring (HBM) project (HBM4EU), PARC has prioritised a set of chemicals for evaluation in years 1-3, with additional prioritisation underway for years 4 onwards. Nanomaterials and advanced materials were identified by several stakeholders as an important priority of focus for the coming years. To facilitate this, and ensure that PARC's efforts enhance ongoing activates (e.g., funded under Horizon Europe, and member states activities) rather than duplicating work, a first step in the process will be to undertake a landscaping exercise and to develop a RoadMap for Nano and Advanced Materials in PARC. As with all major chemical groups and methodologies being addressed in PARC, chemical leads have been appointed to develop the nanomaterials roadmap, and will work with stakeholders, relevant ongoing projects (via the PARC SynNet efforts to drive synergies between PARC and related relevant projects, and beyond) and via the networks of PARC partners, many of whom also work with nanomaterials or advanced materials.

2. Developing the PARC nanomaterials roadmap

Many of the unique properties and applications of nanoscale materials arise from the duality whereby nanomaterials have properties of bulk material (*intrinsic properties*) coupled with properties driven by their highly reactive surface chemistry which are dependent on the nanomaterials surroundings (pH, ionic strength, ion composition, available biomolecules) and are thus *extrinsic* or context dependent properties [2].

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Nanomaterials are defined by their chemistry, size, shape, and surface properties, and by a wide-range of calculated descriptors arising from their elemental composition [3].

The challenges in describing nanomaterials, and making nanosafety research data FAIR arise from a number of sources including: (i) the interdisciplinarity of nanosafety (which spans materials science, chemistry, analytical exposure and toxicology both human and environmental) which results in (ii) an enormous breadth of data types including materials characterisation, environmental transformation and fate and effects data, (iii) the fact that there are many nonstandard (mechanistic-focussed) methods including many which are highly data-intensive such as "omics" and high content screening approaches, (iv) the variety of measurement principles and experimental setups from *in vitro* to *in vivo* to mesocosm and field scale experiments, and (v) the evolving requirements from new research foci such as safe and sustainable by design of materials [4]. Recent example of approaches that require largescale data re-use are materials modelling [5], safe by design modelling of nanomaterials [6], and optimising the safe use of nanotechnologies through re-use of nanosafety data to support the achievement of the UN Sustainable Development Goals [7].

PARC has a number of landscape mappings underway, related to capacities and facilities across PARC partners for example, as well of the data landscapes related to different chemicals. Utilising the methodology and approaches used for mapping of capacities, and building on the experiences of the other Chemical Leads, the PARC nanomaterials leads will establish a working group to perform a landscape mapping of existing nanomaterials and advanced materials knowledge to the PARC activities to identify areas where maximum synergy can be achieved, through collaboration with existing activities and/or through bespoke PARC-led activities to supplement ongoing activities and gap-fill areas where no current activity is occurring and which maps to PARC overarching priorities of regulatory relevance for chemicals risk assessment.

Given the leadership demonstrated by the nanosafety research community in developing tools and solutions to support both FAIR (Findable, Accessible, Interoperable and Re-usable) data and for Safe (and Sustainable) by Design (SSbD), as well as the match of these activities to dedicated efforts in PARC (WP7 for FAIR data and WP8 for SSbD, see also the Tools and Resources section of the PARC website), it is clear that these two aspects will form a key focus for the landscape mapping and synergy development. Demonstration of the translation of research findings from nanomaterials safety and tools developed for nanomaterials to advanced materials research will also be a key focus. All outcomes of the Nanomaterials Roadmap will be made FAIR and open also, in line with the ambition of PARC to make all datasets accessible and reusable for research and risk assessment purposes, as part of an "Open Science" approach that takes into account ethical, legal and confidentiality considerations, following the "as open as possible, as closed as necessary" principle.

3. Conclusions

The initial inputs and prioritisation for the PARC nano- and advanced materials landscape mapping and roadmap for PARC activities will be presented, and

MaterialsWeek participants will have the opportunity to feed into the activity in order to shape the work undertaken in Years 4-7 of PARC and where these can have a strong focus on nanomaterials and advanced materials. A strong focus on synergies (managed through PARC SynNet will also be facilitated via interactions at MaterialsWeek.

4. References

- [1] Marx-Stoelting P, et al. A walk in the PARC: developing and implementing 21st century chemical risk assessment in Europe. Arch Toxicol. 2023 Mar;97(3):893-908. https://doi.org/10.1007/s00204-022-03435-7
- [2] Lynch I, et al. A strategy for grouping of nanomaterials based on key physicochemical descriptors as a basis for safer-by-design NMs. Nano Today 2014, 9(3), 266-270. https://doi.org/10.1016/j.nantod.2014.05.001
- [3] Wyrzykowska E, et al. Representing and describing nanomaterials in predictive nanoinformatics. Nature Nanotechnology, 2022, 17(9), 924-932. https://doi.org/10.1038/s41565-022-01173-6
- [4] Exner TE, et al. Metadata stewardship in nanosafety research: learning from the past, preparing for an "on-the-fly" FAIR future. Frontiers in Physics, 2023, 11, https://doi.org/10.3389/fphy.2023.1233879.
- [5] Yang RX, et al. Big Data in a Nano World: A Review on Computational, Data-Driven Design of Nanomaterials Structures, Properties, and Synthesis. ACS Nano 2022, 16, 12, 19873–19891. https://doi.org/10.1021/acsnano.2c08411
- [6] Furxhi I, et al. A. Data-Driven Quantitative Intrinsic Hazard Criteria for Nanoproduct Development in a Safe-by-Design Paradigm: A Case Study of Silver Nanoforms. ACS Applied Nano Materials, 2023, 6(5), 3948-3962. https://doi.org/10.1021/acsanm.3c00173
- [7] Alfaro Serrano, et al. The role of FAIR nanosafety data and nanoinformatics in achieving the UN Sustainable Development Goals: the NanoCommons experience RSC Sustain., 2024, https://doi.org/10.1039/D3SU00148B