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# The role of FAIR nanosafety data and nanoinformatics in achieving the UN sustainable development goals: the NanoCommons experience†

Beatriz Alfaro Serrano,[a] L. Cristiana Gheorghe,[b] Thomas E. Exner,[c] Susanne Resch,[a] Clemens Wolf,[a] Martin Himly,[d] Andreas Falk,[a] Nathan Bossa,‡[e] Socorro Vazquez,[e] Anastasios G. Papadiamantis,[bfg] Antreas Afantitis,[fg] Georgia Melagraki,[h] Dieter Maier,[i] Haralabos Saramveis,[j] Egon Willighagen,[k] Vladimir Lobaskin,[l] Jonathan D. Oldfield[b] and Iseult Lynch *[bg]

The increasing focus on open and FAIR (Findable, Accessible, Interoperable and Re-useable) data is driving a step-change in how research communities and governments think about data and knowledge, and the potential for re-use of data. It has long been recognised that international data sharing is essential for regulatory harmonisation and commercialisation, *via* the Mutual Acceptance of Data (MAD) principle of the Organisation for Economic Cooperation and Development (OECD) for example. However, it is interesting to note that despite the power of data and data-driven software to support the achievement of the United Nations Sustainable Development Goals (UN SDGs), there appears to be limited awareness of how nanomaterials environmental health and safety (nano EHS) data can drive progress towards many of the SDGs. The goal of the NanoCommons research infrastructure project was to increase FAIRness and impact of nanoEHS data through development of services, including data shepherding to support researchers across the data life cycle and tools such as user-friendly nanoinformatics predictive models. We surveyed both service providers and service users on their ideas regarding how nanoEHS data might support the SDGs, and discovered a significant lack of awareness of the SDGs in general, and the potential for impact from NanoCommons tools and services. To address this gap, a workshop on the SDGs was prepared and delivered to support the NanoCommons service providers to understand the SDGs and how nanosafety data and nanoinformatics can support their achievement. Following the workshop, providers were invited to update their questionnaire responses. The results from the workshop discussions are presented, along with a summary of the 12 SDGs identified where increasingly accessible nanoEHS data will have a significant impact, and the 5 that are indirectly benefited along with some recommendations for EU-funded projects on how they can maximise and monitor their contributions to the SDGs.

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[a]BioNanoNet Forschungsgesellschaft mbH, Kaiser-Josef-Platz 9, 8010 Graz, Austria
[b]School of Geography, Earth and Environmental Sciences, University of Birmingham, Edgbaston, B15 2TT Birmingham, UK. E-mail: i.lynch@bham.ac.uk
[c]Seven Past Nine GmbH, Rebacker 68, 79650 Schopfheim, Germany
[d]Dept Biosciences & Medical Biology, Paris Lodron University of Salzburg, Hellbrunnerstrasse 34, 5020 Salzburg, Austria
[e]LEITAT Technological Center, C/ de la Innovació 2, 08225 Terrassa, Barcelona, Spain
[f]Nanoinformatics Department, NovaMechanics Ltd, Nicosia, Cyprus
[g]Entelos Institute, Larnaca, Cyprus
[h]Hellenic Military Academy, Vari, Greece
[i]Labvantage – Biomax GmbH, Robert-Koch-Str. 2, 82152 Planegg, Germany
[j]Unit of Process Control & Informatics, School of Chemical Engineering, National Technical University of Athens, Greece
[k]Department of Bioinformatics – BiGCaT, School of Nutrition and Translational Research in Metabolism, Maastricht University, Universiteitssingel 50, 6229 ER Maastricht, The Netherlands
[l]School of Physics, University College Dublin, Belfied, Dublin 4, Ireland

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‡ Current affiliation: TEMAS Solutions GmbH, Lätteweg 5, 5212 Hausen, Switzerland.

**Sustainability spotlight**

Despite the strong policy push towards safe and sustainable by design materials and the race to net zero, research communities are not always aware of the potential for their research to support achievement of the UN Sustainable Development Goals (SDGs). Nanomaterials environmental health and safety (nanoEHS or nanosafety) research clearly addresses SDG 3 (good health and well-being) and SDG 12 (responsible consumption and production), given its focus on reduction of human and environmental toxicity of nanoscale materials. Further analysis of the combined impacts of (i) making nanosafety data more findable, accessible, interoperable and re-useable (FAIR) and (ii) the democratisation of access to advanced nanoinformatics through provision of user-friendly models for nanomaterials hazard and risk prediction (that do not require users to have advanced programming skills), *via* community-focussed research infrastructures ("commons") determined that nanoEHS directly supports 12 of the 17 SDGs, and indirectly supports the other 5 SDGs. However, the benefits of FAIR data and software can only be fully exploited when available on public infrastructures like NanoCommons, which are themselves sustainable.



## 1 Introduction

Anthropogenic pressures on the Earth System have reached a scale where abrupt global environmental change can no longer be excluded. Over the last decade, sustainability researchers have determined *planetary boundaries* in order to establish the "planetary playing field" for humanity and reduce the concomitant risk of major human-induced environmental change on a global scale.[1] Transgressing one or more planetary boundaries may be deleterious or even catastrophic due to the risk of crossing thresholds that will trigger non-linear, abrupt environmental change within continental-to planetary-scale systems.[1,2] Nine planetary boundaries have been defined, including climate change, ocean acidification, stratospheric ozone, biogeochemical nitrogen and phosphorus cycles, global freshwater use, land system change, the rate at which biological diversity is lost, chemical pollution and atmospheric aerosol loading. The social impacts of transgressing boundaries will be a function of the social–ecological resilience of the affected societies, and inevitably, less economically developed societies will be more affected than developed economies where even basic needs such as access to clean water and power/energy are not always met. Calculations suggest that while physical needs such as nutrition, sanitation, access to electricity and the elimination of extreme poverty could likely be met for all people globally without transgressing planetary boundaries, the universal achievement of more qualitative goals (for example, high life satisfaction) would require a level of resource use that is 2–6 times the sustainable level, based on current relationships.[3] Thus, innovative approaches are needed to develop sustainable materials, processes and approaches that support improved life quality for all within the planetary boundaries and meet social needs.

Against this backdrop, the 2030 Agenda for Sustainable Development was adopted by world leaders in September 2015 setting an ambitious 15 year agenda to mobilize global efforts to end all forms of poverty, fight inequalities and tackle climate change, while ensuring that no one is left behind, resulting in the 17 SDGs. The SDGs build on, and go beyond, the relative success of the eight Millennium Development Goals (**https://www.un.org/millenniumgoals/**) which were the focus of the global developmental agenda for the 15 years from 2001–2016. As per the UN SDG statement, the SDGs "*recognize that ending poverty must go hand-in-hand with strategies that build economic growth and address a range of social needs including education, health, social protection, and job opportunities while tackling climate change and environmental protection*".

Feeding into the momentum surrounding the establishment of the SDGs, in November 2014 an Independent Expert Advisory Group to the UN made concrete recommendations on bringing about a *data revolution* in sustainable development.[4] The report highlighted two big global challenges for the current state of data: (i) the challenge of invisibility (gaps in what we can discern from the data and the timeliness of the data generation), and (ii) the challenge of inequality (gaps in terms of those who are able to access necessary information in order to make their own decisions) and called for a UN-led effort to mobilise the data revolution for sustainable development through:

- Fostering and promoting innovation to fill data gaps; mobilising resources to overcome inequalities between developed and developing countries and between data-poor and data-rich individuals and groups,§ and
- Leadership and coordination to enable the data revolution to play its full role in the realisation of sustainable development.

Since then, several major initiatives have emerged to support increasing democratisation of access to data, including the Open data movement, *e.g.*, the EC has expanded its demand for research to produce open data), the publication of the FAIR (Findable, Accessible, Interoperable and Re-useable) data principles[5] and more. We note, of course, that FAIR data is not the same as Open data, but by making data FAIR (Findable, Accessible, Interoperable and Re-useable) there is greatly increased clarity in terms of what data exists (*via* the indexed metadata), how to access this data (and from whom permission is needed), and the licence conditions for any proposed re-use thus increasing the potential for effective repurposing of data enabling improved data driven decisions. While progress towards data sharing has generally been quite slow, several promising movements have emerged recently, including the **https://www.un.org/sustainabledevelopment/sdg-publishers-compact/**, which is designed to inspire action among publishers to accelerate progress to achieve the SDGs by 2030; this includes encouraging and promoting articles related to SDGs and acting as champions of the SDGs during the Decade of Action (**https://www.un.org/sustainabledevelopment/decade-of-action/**) (2020–2030) *via* the by removal of paywalls from key articles and related initiatives. Another recent initiative is the Data Values movement which calls for urgent action to create a FAIR data future; for example, the Data Values Project (**https://www.data4sdgs.org/blog/data-values-act-now-create-fair-data-**

§ **https://www.un.org/en/global-issues/big-data-for-sustainable-development**

**future-all**) proposes a new agenda for how data is collected, managed, funded, and used with the aim of helping and empowering people, recognising that data needs to serve everyone, and this is as much a political and social endeavour as it is a technical one. Building on FAIR, recent initiatives for data repositories such as TRUST (Transparency, Responsibility, User focus, Sustainability and Technology)[6] and CARE (Collective benefit, Authority to control, Responsibility, and Ethics) principles for indigenous data governance.[7] There have also been important developments recently in terms of open and FAIR software and research services,[8] which will, in principle, support the uptake and utilisation of data in tackling the SDGs.

In terms of technologies that can be applied to support the SDGs, nanotechnologies have long been recognised as having the potential to offer disruptive, game-changing breakthroughs and innovations that can provide immediate answers and solutions to help our society, environment, and the planet, and to solve many of humanity's grand challenges. Indeed, nanotechnologies potential role in addressing the Millennium Development Goals was evaluated by the United Nations Task Force on Science, Technology and Innovation as far back as 2005.[4] A recent review paper summarised the potential of nanotechnologies to support and drive international efforts in sustainability and to support the achievement of the United Nations' SDGs.[9] The authors suggest that nanotechnologies can accelerate the progress toward the SDGs through technological solutions and interdisciplinary skills in communication and tackling difficult challenges.[9] They identified six key areas for advances, as shown in Fig. 1, including:[1] the Internet of Things (IoT) integrating Artificial Intelligence and quantum devices to bring innovations in computing, which underpins many of the SDGs;[2] transportation with high safety and low environmental impact, utilising for example light-weight yet strong nanocomposite materials addressing Goal 11: Sustainable Cities and Communities;[3] nanobiotechnology for health and medical care addressing Goal 3: Good Health and Well-being as well as Goal 2: Zero Hunger (Food and Agriculture) and Goal 12: Responsible Consumption and Production;[4] service robots coexisting with and supporting people which is linked to healthy ageing and thus Goal 3: Good Health and Well-being;[5] smart materials to enable sustainability of water, air, and materials which addresses multiple goals including Goal 13: Climate Action, Goal 14: Life Below Water and Goal 15: Life on Land; and[6] energy materials and devices to enable renewable energy production and energy saving addressing Goal 7: Affordable and Clean Energy.[9] Underpinning the translation of all of these into real world solutions for the global south is the need for data sharing and democratised access to knowledge.

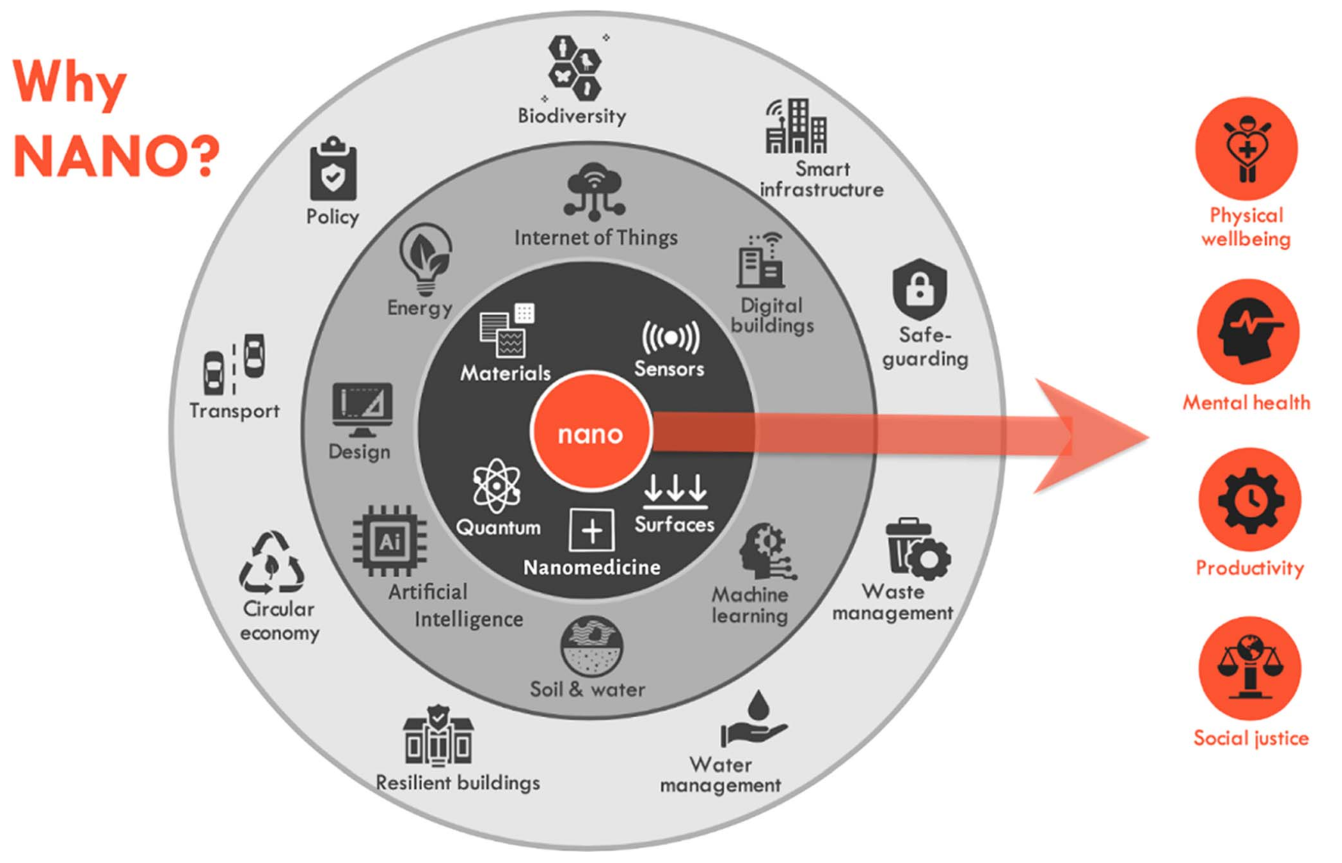


Fig. 1 Nanotechnology is at the core of technology-based solutions for a sustainable future, driving advances in the Internet of things and machine learning, in renewable energy, in enhanced waste management and more, which collectively lead to improved human and environmental health. Reprinted with permission from.[9] Copyright 2021 American Chemical Society.

Indeed nanotechnologies and advanced materials are at the heart of the EU sustainability agenda including the EU Green Deal (https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal_en) which lays out Europe's transition into the first digitally led circular, climate-neutral and sustainable economy, and the Advanced Materials Initiative 2030 (https://www.ami2030.eu/) *via* which safe and sustainable materials provide a backbone and source of prosperity for a sustainable society. However, there is a major challenge to ensure that these advances are achieved in an inclusive manner (a core tenet of the SDGs), and that the application of nanotechnologies does not further exacerbate the technological and informational divide. Recent research on the wider societal considerations of emerging technologies including nanotechnologies, reflects on issues such as economic and social (in)justice, potential violations of privacy and autonomy, and unethical applications.[10] In the face of these ethical issues, the authors argue that there is a need for transparency, interdisciplinary panels concerned with "nano-ethics" and institutions of democratic control (governance and regulation) of technological solutions.[11]

EU-wide research infrastructures, which harness communities and accelerate research in priority areas, have a key role in enhancing the accessibility of research data, tools and services, and in increasing the training in emerging technologies in their domain. As such research infrastructures are playing an increasingly important role both in supporting FAIR data for their research domain, and in enhancing the sustainability and accessibility of the products of research, and thus are ideally placed also to support the translation of research to support the SDGs. The EU-funded starting-community (https://cordis.europa.eu/programme/id/H2020_INFRAIA-02-2020) research infrastructure project NanoCommons (http://www.nanocommons.eu/) (2018–2022) was mandated to initiate the development and implementation of a central, community-wide knowledge infrastructure facilitating the development of predictive models and nanoinformatics tools and the harmonisation and FAIRification of nanomaterials safety data for modelling, safe-by-design product development and regulatory approval. Due to its overarching goal to become the central infrastructure for nanomaterials safety, NanoCommons acts as a role model and best practice example for addressing the sustainability challenges described above. To achieve this, the project aimed to implement and provide its tools and services in a manner fostering economic, environmental and social sustainability directly *via* the transition towards a digitalised and collaborative approach to nanomaterials environmental health and safety (nanoEHS) research and sharing openly and FAIRly the resulting datasets, models and software to allow their re-use globally.

As part of its commitment to sustainability and impact from its activities, NanoCommons performed an evaluation of how its research support services, through provision of access to its data shepherding (FAIR data management) services and its bespoke development of nanosafety informatics tools for prediction of the hazards associated with nanomaterials, are perceived by both *service providers* and *service users* with respect to the "global innovation system" for sustainable development technologies. The extent to which NanoCommons datasets, models and tools can contribute to each of the 17 SDGs throughout the value chain, and the risks and opportunities they individually represent, was analysed based on the survey results, training sessions on the SDGs provided to the service providers, and analysis of the literature. The results of this evaluation are presented, and provide the basis for recommendations on where positive impacts can be scaled up, where negative impacts can be reduced or avoided, and where additional activities or refocusing is needed to target even more SDGs *via* FAIRification of data and informatics tools and software.

## 2 Methods and approaches

### 2.1 Initial mapping of NanoCommons potential to contribute to the SDG

The UN SDGs are intended to be achieved by the year 2030, as per UN Resolution 70/1 setting out the 2030 Agenda (https://sustainabledevelopment.un.org/post2015/transformingourworld), and were designed to be a "blueprint to achieve a better and more sustainable future for all" by addressing and balancing the following three main pillars: economic sustainability (also referred to as *profit*), environmental sustainability (also referred to as *planet*) and social sustainability (also referred to as *people*). The first objective was to map the SDGs onto the NanoCommons activities and outputs to identify which SDGs are the most important, as not all 17 SDGs were expected to be equally relevant for NanoCommons.

### 2.2 Evaluation of the services provided by NanoCommons *via* its transnational access pillar

Within the EU Research infrastructure funding model, research infrastructures should provide "Access" to laboratory facilities and/or computational resources and other services. In the case of NanoCommons, whose focus was on integrating and FAIR-ifying the nanosafety data landscape to facilitate development of nanosafety informatics models (nanoinformatics) the access offered was grouped into 4 categories as shown in Fig. 2: (i) experimental (data management) workflows, (ii) data processing and analysis tools to support the integration, quality assurance, ontology annotation and uploading of data into repositories, (iii) data visualisation and predictive toxicity modelling with a strong focus on predicting nanomaterials properties, exposure and impacts, and (iv) data storage and online accessibility services to increase the availability and long-term preservation of data.

Users, who applied for access *via* rolling and targeted calls for users, were specifically supported by the NanoCommons partners in using the services and adapting them to their specific needs. This was possible through the specific instrument of European infrastructure projects called Transnational Access (TA). In the case of NanoCommons, nanosafety

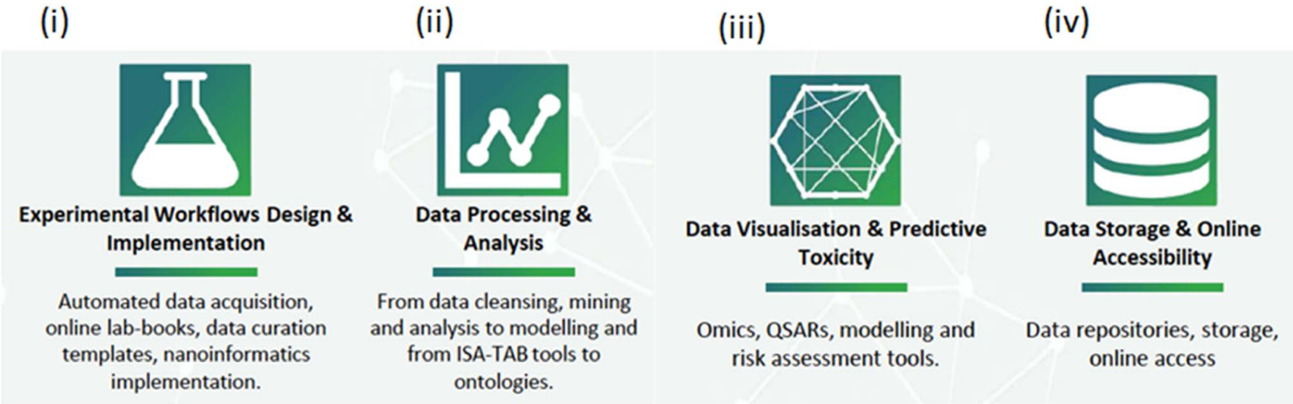


Fig. 2 Categories of NanoCommons services. Note that in (iii) "Omics" is shorthand for omics data analysis pipelines and workflows.



researchers from industry, academia and regulatory bodies were able to apply for TA projects giving them access to the state-of-the-art NanoCommons expertise, services, and facilities free of charge to advance their work, solve problems and take their research to the next level.

### 2.3 Questionnaire for service providers and users

Since the TA projects represent real-world applications of the infrastructure, they were also the best testbed for evaluating if NanoCommons met its goals with respect to boosting sustainability of nanosafety research in general and providing a sustainable data and nanoinformatics infrastructure more specifically. A questionnaire, reproduced in ESI 1,† was sent to all providers and users of the 31 TA projects (see Table S1 in ESI 2†), asking for an evaluation of the TAs from the different perspectives,

(1) Service provider perspectives were focussed on:

(a) The commercial potential of the specific tool or service;

(b) Lessons learned for improving the service;

(c) Relevance for the UN SDGs.

(2) Users were asked to give their perspective on the services they utilised assessing their:

(a) Satisfaction with the TA outcomes;

(b) Interest in future access to these services, potentially in a commercial setting

(c) Views on the relevance of the tool/service for addressing the SDGs.

Not all providers or users completed the survey, so the analysis is based on those that did respond (20 completed TA project teams provided feedback).

### 2.4 SDGs workshop

It was evident from the early replies to the survey of TA project that the providers and users were often uncertain how to relate the work performed and the obtained results to the SDGs, both on an individual TA level as well as on the level of the broader impact of the supported projects and similar projects benefiting from the NanoCommons services. This led to many NanoCommons partners asking for more training on the SDGs. To address this need and to support the TA providers an interactive webinar on SDGs was organised on 9th May 2022. The webinar started with a presentation highlighting the importance of addressing the SDGs with our research and to increase the consortium's knowledge on the different aspects addressed by the SDGs within the nanosafety community. This was followed by an interactive open discussion. An online white board, MURAL (https://www.mural.co/), was used to facilitate the interaction of all NanoCommons partners and to stimulate their active participation while answering the following questions (Q):

- Q1: Which UN SDGs are relevant for NanoCommons from your point of view? How do open/FAIR data, tools and models support the SDGs? What are potential barriers and challenges?
- Q2: How can open and FAIR data, tools and models support the achievement of specific SDGs?
- Q3: What is needed to make 1 + 2 happen?

This created a common understanding on the term "sustainability", put sustainability and the SDGs into a wider context, and created awareness and understanding regarding how open and FAIR data, tools and models supports the achievement of the UN SDGs. The additional knowledge was then put into action by revising the SDG questionnaires of the previous section.

### 2.5 Supporting sustainability and the SDGs *versus* becoming self-sustaining

Running in parallel to the analysis of how FAIR data supports and easier access to nanoinformatics tools can support the SDGs and enhance the sustainability research was an underlying question of whether embedding the services as tools for achieving the SDGs might also serve to enhance the long-term sustainability of the tools and services themselves. Thus, this work was carried out as part of our overall set of activities designed to ensure the legacy of NanoCommons beyond its funded lifetime, considering the 'valley of death' for many pre-commercial research outputs. One of the approaches trialled within NanoCommons to support longer-term sustainability was through building critical mass and a "commons" approach, by integration of tools and approaches developed in previous projects, such as the GUIDEnano decision support tool. Another approach evaluated was providing a common data interface to enable effective integration of data from different databases *via* a semantic interoperability layer that maps the data models in the different databases to identify synonyms to group comparable data. Some of these approaches were more successful than others, but none completely negated the need for sustained investment in resource maintenance and onward development as a community-focussed research infrastructure platform.

# 3 Results and discussion

## 3.1 Overall relevance of "FAIR data"-focussed research infrastructures for the SDGs

In order to evaluate (i) how NanoCommons has been supporting the achievement of the SDGs through its research support services, (ii) how these services are essential for development of safe and sustainable nanomaterials (NMs) and nano-enabled products and, (iii) more broadly, how these services may have a positive impact on the "global innovation system" and the sustainable development of new technologies, the designed questionnaire to evaluate the effectiveness of the TA services provided by NanoCommons was sent to both the TA providers (partners in NanoCommons) and the TA users (the recipients of the NanoCommons services and tools) following the completion of the TA projects. Fig. 3 shows the main SDGs extracted from the first set of completed questionnaires received (*i.e.*, after the first set of TA projects were finalised and reported), mapped to the 3 dimensions of sustainability (people, profit, planet). Interestingly, despite the nanoEHS focus of the project and its services and tools, SDG 3: good health and well-being was not initially identified as one of the SDGs the project was supporting, while SDG 12: responsible Consumption and Production was. Others identified at this stage reflect the collaborative nature of the TA projects (SDGs 16: strong institutions and 17: partnerships) and the infrastructure aspect also emerged, *via* SDG 9.

The SDGs identified in the initial round of TA evaluation are highly relevant for the safety and regulatory aspects of nanomaterials, which aligns with NanoCommons' goals of preventing negative effects from nanomaterials on human health and the environment, as well as highlighting the community-building efforts represented by NanoCommons as a research infrastructure project. However, only 50% of all SDGs were identified as benefiting from NanoCommons activities. It was assumed by the NanoCommons sustainability team that the reason for not considering the other SDGs was not a lack of relevance of our activities but rather a low awareness and knowledge about the SDGs in the NanoCommons consortium and the TA user base. Indeed, both TA service providers and users expressed a need for additional guidance and to help them to place their projects into this larger context when filling in the questionnaire.

To provide this guidance, an internal NanoCommons SDG workshop was organised in May 2022 and the learnings from the workshop were included in the subsequent evaluations of the NanoCommons TA projects. The workshop guided NanoCommons partners through different questions to create a common understanding of the term "sustainability", to place sustainability and the SDGs into a broader context, to create awareness and understanding of how open and FAIR data, and nanoinformatics tools and models support the achievement of


Fig. 3 SDGs mapped onto the three pillars of sustainability that were mentioned in the first set of answers received, either directly or indirectly supported through the research and development activities of NanoCommons. (A refined version of this figure, resulting from the further SDG mapping described below, is provided as Fig. S1 in ESI 3†).

the UN SDGs, and to define potential barriers and challenges. Partners were able to reflect and provide feedback on how concretely their tools developed within the NanoCommons project support the achievement of the SDGs, either directly or indirectly. Together, we developed suggestions on what would be needed to achieve greater impact from, and long-term sustainability of, NanoCommons results. To create an interactive atmosphere in the workshop, an online whiteboard tool was used (Mural), and the whole mural can be seen in Fig. 4 and is accessible online here (**https://www.bnn.at/wp-content/uploads/2023/03/NanoCommons-SDG-Training_2023-03-07_14-14-05.pdf**) to allow zooming in.

The framing of the workshop suggested that as all our activities within NanoCommons were focussed around supporting nanoEHS, some of the SGDs were inherently relevant, such as SDG 3: good health and wellbeing, which positively influenced how participants framed their responses and the subsequent discussions. The organisers pointed to other relevant goals (SDG 10: reduced inequality, SDG 11: sustainable cities and communities, SDG 12: responsible consumption and production and SDG 16: peace and justice *via* strong institutions) prompting discussions around their relevance and the extent to which they are addressed by the NanoCommons services. The open science and data efforts of NanoCommons were identified as being strongly related to all these SDGs since model and data transparency supports good decision making and governance, leading to more sustainable nanomaterials on the market. In addition to the workshop, 1-to-1 sessions were organised with the TA providers, which helped NanoCommons partners to think more broadly and better understand and identify SDGs for which their research outputs could be relevant.

These discussions had a strong influence on the subsequent TA evaluations. Fig. 5 shows the breakdown of the SDGs that were identified based on the combined TA providers and TA applicant perspectives and their mapping onto the three pillars of sustainability is provided in Fig. S1 of the ESI 3.† Now, 12 of the 17 SDGs are selected as relevant at least once. Some SDGs like SDG 3 "good health and well-being" and SDG 6 "clean water and sanitation" are quite obvious and are selected very often since they are directly related to nanosafety. However, it is very encouraging that SDG 17 "partnerships for the goals", was actually the most often named SDG, with SDG 9 "industry, innovation and infrastructure", and SDG 8 "decent work and economic growth", and to a lesser extent SDG 10 "reduced inequality" and SDG 11 "sustainable cities and communities" also being identified frequently in the TA project evaluations. This demonstrates that NanoCommons was successful in its

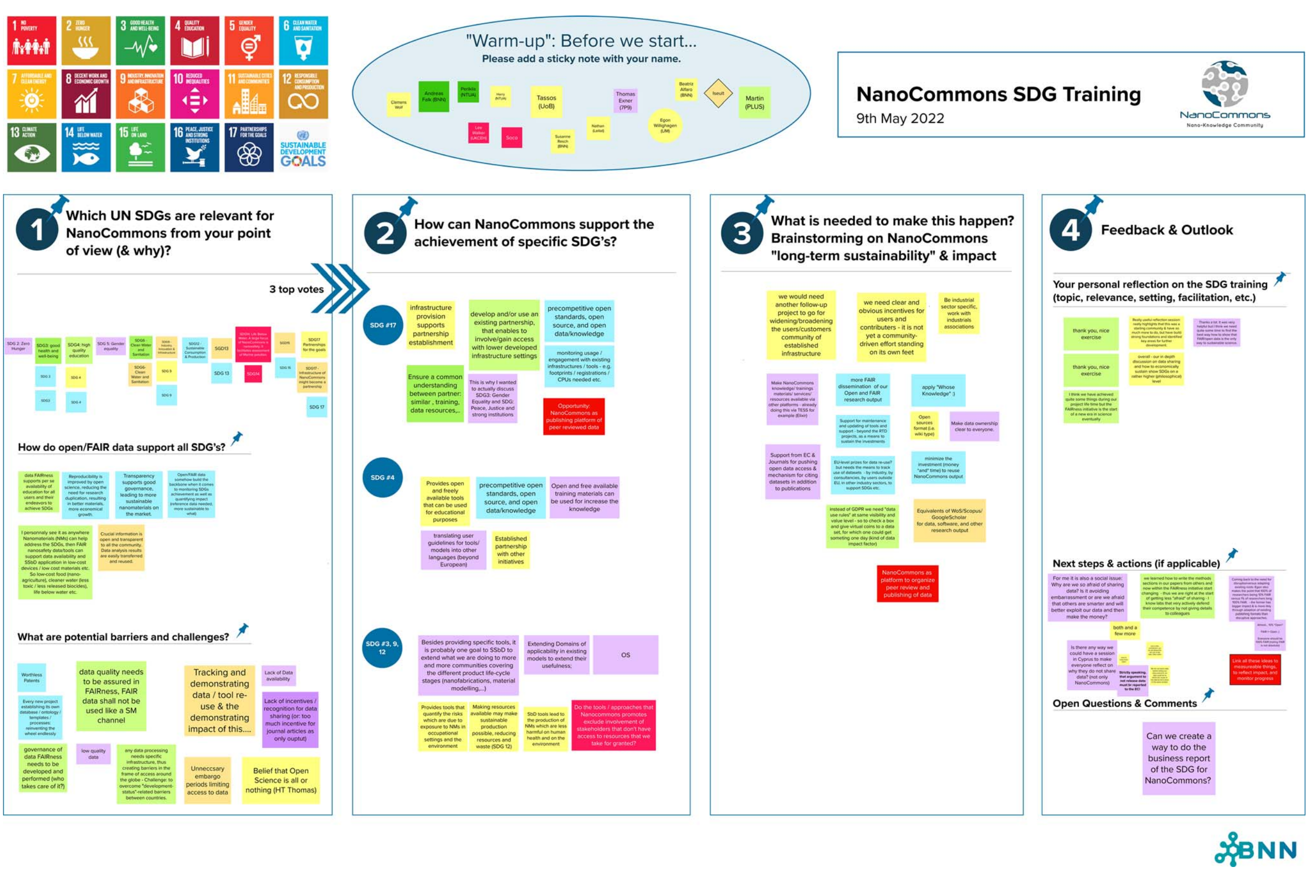


Fig. 4 MURAL board summarising the outcomes of the internal workshop addressing the UN SDGs – readers can access the online version here (https://www.bnn.at/wp-content/uploads/2023/03/NanoCommons-SDG-Training_2023-03-07_14-14-05.pdf) in order to zoom in to the details.

 

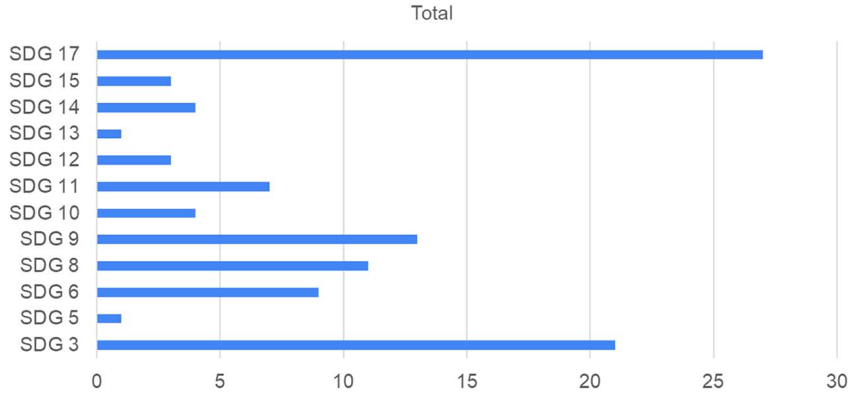


Fig. 5 SDGs identified as being addressed in the different NanoCommons TA projects (based on the TA evaluations from the TA applicant and TA provider perspectives). The $x$-axis shows the number of times an SDG was mentioned in the feedback questionnaires.

mission of being a community building initiative and in providing a nanosafety data and nanoinformatics infrastructure available to many.

Less obvious SDGs were also associated with the TA projects in the revised evaluations, which can be reasoned by the greater awareness of these goals generated in the NanoCommons SDG workshop and more generally by the many journals increasingly tagging articles with specific SDGs. Besides RSC Sustainability as a dedicated journal for this topic, Elsevier have published special issues dedicated to specific goals, and established a tracker for the number of publications addressing each goal over the previous month, while Springer Nature has an SDG programme and communities and recently conducted a survey of researcher attitudes towards each of the SDGs. The raw data from the latter is available for download for further analysis. Most publishers have signed up to the SDG Publishers Compact which aspires to develop sustainable practices and act as champions of the SDGs during the Decade of Action (**https://www.un.org/sustainabledevelopment/decade-of-action/**) (2020–2030), publishing books and journals that will help inform, develop, and inspire action in that direction. We hope that publishing the NanoCommons analysis on how open and FAIR nanosafety research supports the SDGs will give another push to national and EU-funded projects and infrastructures to consider how they can support the achievement of the SDGs.

As an infrastructure project, NanoCommons's mission was the creation of partnerships, promotion of the use of pre-competitive open standards, sharing open science and data/knowledge and integration of solutions (from any source) which are then provided together with open and freely available theoretical and experimental background information and training materials in a single platform to facilitate quality education (SDG 4). The infrastructure "provides open and freely available tools that can be used for educational purposes" and by providing "precompetitive open standards, open source, and open data/knowledge" as per quotes from the Mural board. NanoCommons also covered different life-cycle stages of materials, which contributes to the UN goal of sustainable production and reduction of resources and waste. Safe-by-Design (SbD) and Safe-and-Sustainable-by-Design (SSbD) models should guide the production of NMs which are less harmful to human health and the environment (SDG 3). The infrastructure "provides tools that quantify the risks which are due to exposure to nanomaterials (NMs) in occupational settings and the environment" and "SbD (safe-by-design) tools lead to the production of NMs which are less harmful to human health and to the environment", as reflected in the Mural board.

We recognise that the stakeholder group involved in these discussions represented only a snapshot of the broader nanotechnologies and advanced materials communities. This ensured that the selections were biased towards areas of particular interest and limited by the specific knowledge and understanding of the group. To help address this lacuna, we briefly indicate how nanoinformatics and FAIR data might support the remaining SDGs. For example, as a key enabling technology, nanomaterials are core to innovation and industrial competitiveness, and when applied to develop focussed solutions to local challenges can be a means to stimulate economic activity and provide jobs, thus helping to address poverty (SDG1: no poverty), although access to data regarding safety and sustainability remains essential. In terms of SDG2 (zero hunger), nanotechnologies are being actively developed as carriers for pesticides, fertilisers and to enhance nutrient uptake and as a route to sustainable and precision agriculture. Furthermore, nanoinformatics approaches and access to FAIR data will support the tailoring of solutions for specific soil and climate conditions. With respect to SDG4 (quality education), the combination of nanoscience's central role addressing urgent interdisciplinary socio-environmental issues allied to the innovative democratising dynamic embedded in FAIR data and nanoinformatics web applications promises to provide a stimulating context within which to advance 'inclusive and equitable quality education and promote lifelong learning opportunities for all'. Nanomaterials are core to the development of renewable energy solutions including effective capture and storage techniques in addition to artificial photosynthesis processes, with nanoinformatics and materials modelling offering opportunities to design and test (*in silico*) potential solutions prior to producing them, thus reducing risk and driving progress towards SDG7 (affordable and clean energy).

Finally, the governance of new technologies is essential to ensure that they are developed safely, equitably and sustainably, and nanotechnologies have been at the forefront of responsible innovation and consideration of governance needs. FAIR data will support the transfer of knowledge on responsible governance alongside the channelling of novel applications and help support the establishment of strong institutions essential to SDG16 (peace and justice, strong institutions).

Achieving long-term sustainability of the outputs, beyond the funded project lifetime is a challenge. To achieve sustainability of the NanoCommons Infrastructure and support progress towards the UN SDGs, several community-level recommendations were identified during the workshop as follows:

● Strive for a mixed publicly funded/commercial platform to expand and consolidate the already established infrastructure for users/customers/community and thus also contribute to the establishment of NanoCommons as a publication platform for peer-reviewed data.

● Aim for support from the European Commission & Journals to push for open data access & for a mechanism for citing datasets (in addition to publications), to drive data re-use.

● Sustain EU and project partner's investments in R&D projects by supporting the maintenance of the project outputs (infrastructure, helpdesk, tools, services, *etc*).

● Elaborate incentives for users and contributors, especially the industrial sector, to further grow the FAIR and Open NanoEHS and SbD/SSbD community.

● Provide NanoCommons services and resources, such as shared knowledge and educational materials, through relevant platforms and further emphasise the dissemination of our open and FAIR research results by promoting transparent data ownership, ensuring that the source(s) are acknowledged, and thus strengthening trust in NanoCommons and more generally in the value of the "Commons" approach to sustain community resources.

The FAIR data principles can themselves contribute to sustainable development in a number of ways. For example, they can be used to support the monitoring and evaluation of SDGs, by making data available in a way that allows it to be easily discovered, accessed, and used by stakeholders such as policymakers, researchers, and end-users. Additionally, FAIR data also strengthens sustainable development decision-making and planning by providing reliable and up-to-date information on key indicators and trends. Furthermore, FAIR data can help to support transparency and accountability in sustainable development efforts by making data available to the public and other stakeholders. However, the workshop still left some open comments and challenges with the central question of how to overcome the social problem of fear of sharing data and how to find the best way to show that FAIR/open data is the only path to sustainable science. One highly promising development in this direction, which is building in part on the NanoCommons findings, as well as those from several other research domains, is the WorldFAIR project (**https://worldfair-project.eu/**), which is showcasing a set of 11 disciplinary and cross-disciplinary case studies to advance implementation of the FAIR principles and, in particular, to improve interoperability and reusability of digital research objects, including data. While the focus of the WorldFAIR project is quite technical, in terms of developing and documenting the available best FAIR practice in each research domain, these best practice guidelines are expected to support a transition within and beyond these communities to a greater implementation of FAIR data management. Within each of the case studies, there is also an effort to capture examples of real world practice-change, and of knowledge-enhancement resulting from increased access to FAIR data, and in the nanomaterials case study (**https://worldfair-project.eu/nanomaterials/**), also to increasingly democratised access to FAIR models and software through provisions of user-friendly graphical user interfaces. We note also the important roles of funders and publishers in driving the transition to FAIR and Open data, including *via* the many ongoing initiatives linked to the SDGs, as described in the introduction to this manuscript. Additionally, ongoing training needs (both in terms of using/accessing data in existing repositories, and uploading data to trusted repositories has been identified as a major need within the chemicals risk assessment domain (represented by the EU's Partnership for Assessment of the Risks of Chemicals (PARC (**https://www.eu-parc.eu/thematic-areas/building-infrastructure-and-human-capacities/skills-development-fairification-parc**)), for example). Finally, the key features needed for ideal data repositories (metadata control, data traceability, security, stable infrastructure, and data use restrictions) have been identified based on focus groups which should increase confidence of users in depositing data early and often.[12]

### 3.2 Value of specific research infrastructure services (FAIR data and nanoinformatics tools)

From the global view on the potential contributions of FAIR data-focussed research infrastructures to achievement of the SDGs, we zoom into the specific services provided by NanoCommons, in terms of their contributions to achievement of the SDGs. For this, we will separate the services provided by NanoCommons into two groups, nanoinformatics services (*i.e.*, support from experts in NanoCommons to develop bespoke computational models *via* TA categories (ii) data processing and analysis and (iii) data visualisation and predictive toxicity as shown in Fig. 2) or support for data handling and FAIRification (*i.e.*, services related to topics (i) experimental design and (iv) data storage and online accessibility as shown in Fig. 2).

Many of the nanoinformatics services requested by the first group of users were already quite mature at the start of NanoCommons. Therefore, it was important to see if the infrastructure and its approaches towards harmonisation, interoperability and openness are actually providing additional benefits to users, in part through sustaining access to, and support for, the services. This was accessed by the first set of questions in the questionnaire (see ESI 1†) on the relevance of the NanoCommons Knowledge Infrastructure for sustainability. Somewhat surprisingly but encouragingly, the importance of providing the services as part of an infrastructure was seen as high or very high by all users and providers. Evidence for the importance of research infrastructures to achievement of SDG 17: Partnerships, SDG 9: Industry Innovation and Infrastructure, and partly SDG 8: Decent work and Economic Growth is provided in the following (anonymised) statements from the questionnaires:

- "*The development of such tools promotes the collaboration between experimentalists and computational scientists, maximising data exploitation and the added value from scientific research.*"
- "*The NanoCommons infrastructure supported the collaborative research performed in this TA (project).*"
- "*Adaptation of the existing services to the requirements of the user (TA applicant) along with the offered consultancy functioned as a matchmaking tool to bring the TA applicant and provider together.*"
- "*Such tools can assist with calculating NMs' descriptors in different environments and for computing missing data and helping with the development and regulatory requirements of new materials. They also promote collaboration between experimentalists and computational scientists. Both partners have benefited from each other's expertise, and we will continue our collaboration.*"

Reflecting on the scientific questions and the specific services used in the TA projects, additional SDGs were mentioned. These were mainly SDG 3: Good Health and Well-Being, and SDG 6: Clean water and Sanitation as the main targets of nanosafety research nicely, The following (anonymised) statements expressed the need to guarantee good health and well-being by providing information on the safety of (nano) materials and to support decision making:

- "*This TA application is related to the kinetics of nanomaterials and the translocation rates of NMs into the bloodstream, which might support novel medical research.*"
- "*Having a hub of physiologically based pharmacokinetics (PBPK) models that can easily be integrated into computational pipelines promotes research related to human health. For nanomaterials in particular, there are only a few models that describe their kinetics and especially their translocation into the bloodstream after inhalation exposure, and therefore, having such a model uploaded on a publicly accessible platform is essential for future research on risk mitigation efforts.*"
- "*Predictive models are very important and support the process of designing safer NMs, which maintain the desired functionalities but reduce hazards and adverse effects on human health. The naïve Bayes model will be very useful also in prioritising experimental testing.*"
- "*Predicting the zeta potential of NMs can help with cleaning water from heavy metals.*"
- "*The NanoCommons services were used to bring safe-by-design aspects into a ligand screening campaign to speed up the drug development process. Such collaborative research projects will also in the future be captured, and support in developing customised but still harmonised (meta)data reporting templates and training on how to fill those in.*"

The second group of TAs, which were designed to *support (meta)data curation, ontologies and semantic annotation, and data warehousing*, show a different picture. Firstly, we have to state that the dataset for this group is quite small, since only four TAs were evaluated and of those only two TA applicants answered the question on the received benefits – we expect that this is, at least in part, a reflection of the less clear link between data itself and the SDGs, compared to that from models. Indeed, the ongoing limited understanding of the inherent value of well-described (by rich metadata) datasets and thus of the services to implement metadata and data management, is a major driver for the current article which aims to increase awareness of the role of FAIR nanoEHS data for the SDGs.

We note that in these data curation TA projects the applicants frequently requested ontology or data storage services. However, in the discussions between service providers and applicants it became clear that other more fundamental issues needed to be addressed first, such as supporting the user in defining the metadata (data about their data). This can be collectively termed *data consultancy services* or *data shepherding services* as outlined in [13]. However, these are extremely work intensive, which resulted in most of these TA projects requiring much more time than originally planned. In one case, the applicant withdrew upon understanding the required effort from their side, reflecting on a common misunderstanding that data management can be done "*for you*" rather than "*by you*". It is clear that there remains confusion and misunderstanding of the various roles in the quest to implement the FAIR data principles for nanosafety research data. Database providers, data stewards and data infrastructures like NanoCommons only provide part of the solution, whereas good data management practices have to be implemented at the study design stage and continued throughout all stages of the data life cycle as outlined in [13]. Data shepherding services, as provided by NanoCommons, were an important and appreciated part of the NanoCommons Knowledge Infrastructure services as can be seen from an (anonymised) quote:

- "*Infrastructures are partly technical but for a large component also about human interaction. NanoCommons has acted a "commons" where ideas are exchanged, e.g., via the monthly* NanoSafetyCluster WG-F (**https://www.nanosafetycluster.eu/nsc-overview/nsc-structure/working-groups/wgf/**) *conference calls, as well as the NanoCommons initiatives like the European Registry of Materials,*[14] *the ontology, and the NanoCommons collaborations with the ELIXIR Toxicology Community.*[15] *NanoCommons as a "commons" has created a platform to help researchers unite their research.*"

Similar to the nanoinformatics tools, the SDGs most often mentioned for this group of TA projects are SDG 17: Partnerships, SDG 9: Industry Innovation and Infrastructure, and partly SDG 8: Decent work and Economic Growth, as well as SDG 3: Good Health and Well-Being. While not mentioned in the answers, we want to add SDG 10: Reduced Inequalities, here. All of these benefits are only possible when guaranteeing open access to knowledge, extractable from the data in a collaborative scientific environment.

The experiences from NanoCommons "access" projects show that the high-level project goals have to be aligned and balanced with the shorter-term goals of users, especially those from small and medium enterprises (SMEs) who are often under financial and cash-flow pressure. A key message from users was that data management for its own sake is not sufficient but needs to lead to new opportunities based on data accessibility and re-use. This will take some additional time to demonstrate but inevitably not all datasets will (or should) be reused. A key challenge will be helping users to determine which data have external value and convincing them that concepts and approaches of high-quality data management and data FAIRness are worth implementing also for internal data use and reuse.

It is interesting to note that the differences between data-related and nanoinformatics TAs can even be seen in one single TA. This TA covered a large spectrum of services from data curation of the experimental data, prediction of nanomaterial coronas, to storage of the combined experimental/*in silico* data in the data warehouse (and resulted in a collaborative publication – see [16]. While the objectives of the nanoinformatics part were completely achieved or even overfulfilled by improvement of the model using the experimental data, the full integration of the dataset into the NanoCommons KnowledgeBase was hindered by missing ontology terms and could only be partially realised. This highlights the need for long-term sustainable support for key community-based tasks, such as extending the community ontology coverage on an ongoing basis, to be performed by a central infrastructure.

### 3.3 Balancing commercial and social sustainability goals

Despite the widespread agreement that a nanosafety infrastructure has to be sustained, the answers to the questionnaire also made clear that this cannot happen solely by commercialising the services. This is true for both groups of services (nanoinformatics and FAIR data services) but is especially true for the data services. Even though the NanoCommons KnowledgeBase is based on a commercial data warehouse, running it as a commercial service would only be possible by charging fees to cover the maintenance costs and allow small modifications to follow new scientific developments. The important *data shepherding* costs (*i.e.*, the time spent understanding the users' needs, reaching consensus on what metadata to collect and developing the templates, as described in the very nice series of papers from the Horizon 2020 ASINA project (**https://www.asina-project.eu/**) who were one of the first projects to be guided through the whole process of FAIR nanosafety data management by the NanoCommons data shepherds – see [17–19] could still not be covered by these fees. To use additional (anonymised) quotes from the questionnaire responses:

- *"The commercial potential is low: the cost to the provider is high, translating into a high cost/price for the offer, typically too high for most people (limited research funding, grant funding rules, etc), setting a small potential client base."*
- *"Potential commercial activity will be to receive funding in order to curate the data and metadata from large datasets that cannot be used [currently] in models and tools. Not sure if there is a market for industry or institution."*

Even if possible financially, such a solely commercial sustainability model would not align with NanoCommons' major objective of creating a "commons" for nanosafety research. Additionally, it would contradict the EU initiatives of open data and open science and would prohibit having any positive impact on SDG10: reduced inequality by restricting access to those who can pay. Getting more and more data publicly available (and with a clear re-use licence) along with technical infrastructure development is needed, as one TA provider explained:

- *"Downstream markets depending on (open) data, such as markets involved in computational toxicology and Integrated Approaches to Testing and Assessment (IATA) will benefit from this work. Commercial potential can be found by providing dedicated application programming interfaces (APIs) to make processing this data easy/easier for clients by integration into their platforms. With open data more easily flowing between data hosting providers, all hosting providers have more freebies to offer to clients to show the power of their platforms and application programming interfaces (APIs)."*

This knowledge and data have the potential to lead to many innovations and to economic growth, but only if it is provided in a way that others can use it, meaning in an open and FAIR way. Therefore, it should be the goal of everyone to contribute to data management in their specific role and this has to be acknowledged by reserving meaningful funds in all publicly funded projects for data curation and data shepherding work, as implied by the comments above, and by providing additional funds for the central infrastructure, especially with new challenges arising from the needs of advanced materials in a circular economy. This will have an immense impact on many of the UN SDGs, including some not mentioned in the analysis above. Reducing inequality (SDG 9) was already mentioned, but also SDG 11: sustainable cities and communities, SDG 12: responsible consumption and production, SDG 13: Climate action, SDG 14: Life below water, and SDG 15: life on land, are already profiting from services provided by NanoCommons, albeit in a more indirect way. Participants of the TA evaluation questionnaire focused mainly on the direct impact of their technical work and/or data and their awareness of other sustainability aspects might still be low. Thus, insufficient, and missing knowledge about social, environmental and economic sustainability goals might be the reason why their importance has not been reflected in the TA evaluation questionnaires, which needs to be addressed by additional training, similar to the one provided to the NanoCommons team (the service providers).

All TA providers and user agreed that the NanoCommons services provide important solutions and play a significant role in reaching social and environmental SDGs, either directly or indirectly *via* the results achieved by the research projects the TAs supported, and that this is the reason for the importance to sustain the infrastructure in the future. SDG 3: good health and well-being, SDG 6: clean water and sanitation, SDG 10: Reduced Inequalities and/or SDG 17: Partnerships are mentioned in almost all evaluations. Some additional (anonymised) quotes from the questionnaire are provided here as user testimonials:

 

- *"Some of our samples are intended for modification of membranes for cleaning water and antibacterial, antiviral applications."*
- *"Certainly the integration of in silico modelling procedures into experimental in vitro workflows will allow us to counteract existing data gaps in nanosafety assessment. In addition, this TA contributed by improving data FAIRness to SDG 3. In addition, the developed in silico techniques can be used to support product optimization for nanomedicine."*
- *"EU-financed open access, FAIR data reflect an enabling data donation to the global community."*
- *"It enables easier data sharing for research on manufactured and incidental nanoparticles in the environment, including: drinking water sources (SDG 6), aquatic environments (SDG 14), and soils (SDG 15). The effects of data sharing are likely to lead to further insights on potential harm as well as protection measures of nanoparticles in these environments."*
- *"I was very impressed with NanoPharos database's collection of high-quality data. It made the development of in silico alternative testing strategies a lot easier and more efficient. Thanks to NanoPharos, we were able to save time and resources while improving the safety and efficacy of our nanomaterials*."

A few of the TA users considered the commercial options for the provided services, even if the amount they would be willing to pay for such services is considerably below the costs for running the TA or they were not able to estimate acceptable amounts at the current state. Corresponding statements[20]

- *"Developing a new methodology is a scientific process that cannot be directly linked to commercial activities, at least at its early stages. However, the re-estimated cost that is related to consulting activities around the use of the new estimation method is reasonable."*
- *"The actual cost for deploying a physiologically based pharmacokinetics (PBPK) model on* Jaqpot (**https://www.jaqpot.org/**)[20], *offered via NanoCommons, is reasonable. The service could be requested in a commercial setting."*
- *"Currently such costs for FAIR data are mostly not budgeted into projects, but would need to be done in future, in agreement with scientific journals [who are] more and more demanding data FAIRness; in silico-in vitro experimental correlation and vice versa data enrichment is in its infancy at present. If such workflows become more often used, projects may start budgeting costs for it that may be outsourced to e.g., a commercial NanoCommons infrastructure."*
- *"Enalos Cloud Platform allowed us to do that [develop models] without requiring a deep understanding of the underlying technology. The platform's pre-built models and algorithms were incredibly useful, and we were able to quickly develop and deploy predictive models that helped us make data-driven decisions. Certainly cheaper than contracting modellers".*

We would argue that, because of its many benefits for the social and environmental SDGs, the core infrastructure and services around FAIR data management and nanoinformatics provision are not intended to become a commercial product but rather should provide an open innovation platform to facilitate achievement of the SDGs and be partly complemented by commercial services.

### 3.4 Demonstration cases to accelerate transfer of technical support to the SDGs

While the "Access" projects were successful in solving issues on a local (institutional or project) level, they highlight the need for further community building and knowledge exchange to address major global challenges like (a) the current insufficient amount of data and low data completeness for re-use in specific contexts such as for regulatory risk assessment, (b) the high workload involved in data sharing currently and (c) the limited or missing regulatory acceptance of nanoinformatics approaches currently. These challenges require concerted community effort over a sustained period (years) to drive changes in mindsets, develop tools for automation of data curation and management, and to progress nanoinformatics through model validation processes to have them recognised as alternative test methods. The NanoCommons Demonstration Cases (**https://nanocommons.github.io/user-handbook/demonstration-cases/**) were designed to identify such long-term developmental needs and to demonstrate how a central infrastructure can support and accelerate these developments. Providing support to the SDGs was one of the main selection criteria for the Demonstration Cases. A short description of the objectives of four of these cases is presented along with a description of how they relate to specific SDGs.

Two of the demonstration cases relate to SDG17: Partnerships (collaboration) and SDG 16: Strong Institutions (supporting Governance & Justice):

- NanoCommons was designed to build the community infrastructure for nanosafety research in all its aspects and diversity. However, many other projects *e.g.*, nanoinformatics, Safe-by-Design, governance, nanofabrication calls, which are developing tools, services and even platforms and portals. To avoid these becoming silos, developing tools in isolation that cannot be integrated or sustained over the long term, and to prevent fragmentation of nanosafety data and simultaneously achieve a harmonisation of data, a demonstration case was created to start collaboratively defining general interfaces for interoperability, core e-infrastructure components and to solve legal issues to preserve confidentiality and IP rights. The goals were to [1] establish a neutral approach to support harmonisation, interoperability, sustainability and to foster a community development/collaborative approach to co-develop a robust set of complementary solutions to support the range of stakeholders needs,[2] support clusters of projects funded under the same or related calls through networking and brokering activities, identifying key areas where some "bridging" resources are needed to allow cross-talk and make the whole nanosafety ecosystem much more than the sum of the individual parts (projects), and[3] collate and document all relevant training activities in one place, showing the progress of the area by giving access to the news but also older materials, and fostering synergies between and avoiding duplication of training activities. Strengthening the community by active knowledge exchange and improved interoperability will clearly have a positive effect on all SDGs but SDG 17: Partnership and SDG 4: Quality Education, clearly stand out as the ones defining this demonstration case. While SDG4 was discussed in the SDG workshop, it was not associated with a specific TA (see Fig. 5) since it requires more than is possible to fulfil in one TA.

● Regulatory agencies encourage the use of alternatives to animal testing and specifically the use of *in silico* methods. However, very few such methods that are accepted/endorsed by regulatory agencies, and none are for nanomaterials – no nanoinformatics workflows have been accepted for use in regulatory assessment as yet. To support researchers in building regulatory acceptance for models and tools, a short- and long-term roadmap is needed. Although the demonstration case was only able to work on reporting standards, it was the start to establish the process(es) for gaining regulatory acceptance of nanoinformatics models (both data-driven such as quantitative structure–activity relationships (QSAR), PBPK models, *etc.*) and physics-based models (*e.g.,* materials models, binding affinities, and corona formation). This will be continued in subsequent projects by working through the various processes such as submitting models to ECVAM (established for QSAR models and some initial ECVAM activity around PBPK models), submitting selected models to the OECD Approaches to Testing and Assessment (IATA) case study project (as part of Nano-SolveIT) and/or establishing a CEN Workshop Agreement. In the long run, we envisage that this will lead to regulatory-accepted, high-quality models and *in silico* tools allowing high-confidence assessments of many more materials. More informed policy decisions can then be made supporting SDG 16: Peace and Justice Strong Institutions.

Two other demonstration cases were started to support open science by improved documentation and knowledge sharing.

● Laboratories have a lot of inherent knowledge on how to design and implement a study, which is transferred from one generation of co-workers to the next or from the principal investigators to their co-workers. However, since this knowledge is often not documented on paper or electronically, it cannot be used outside the one laboratory to train researchers as early as at the undergraduate level. Nor can these in-house practices be evaluated to check if the process complies with state-of-the-art quality criteria and check how it compares to processes established in other laboratories. Therefore, one demonstration case defined a way to document the study design process in specific laboratories with respect to the decision-making process applied. This was combined with approaches to use the study design as the basis for organising the data collection and management processes, the integration of quality assurance and control measures and their documentation, and to pack all of this into a publicly shareable information resource.

● Performing experiments following standard operating procedures (SOPs) is essential in industrial settings to guarantee reproducibility and in regulatory settings for validation of the method and acceptance of the result and conclusions. SOPs are now also more and more implemented in basic- and early-research academic and industrial laboratories. Developing these SOPs is a complex and time-consuming process, but it is rarely documented with respect to the thought processes, which went into the SOP, and quality assurance measures adopted during the development. Additionally, SOPs are in most cases only shared if absolutely needed *e.g.,* for regulatory validation and even if they are, the free-text format makes independent quality control and comparison of different SOPs almost impossible. Therefore, another demonstration case was created to provide standard ways of documenting the SOP development process and derive a checklist for assessment of SOP quality and completeness. Similar to the previous case, all this information can then publicly be shared giving others the chance to perform experiments to these high-quality standards or apply the learnings to their own methods for quality improvement and assurance.

This ongoing effort to support open knowledge and expertise sharing will allow the global community, including areas not able to perform expensive developments and long validation studies, to build upon the FAIR nanoEHS datasets and models. This will strengthen SDG9: Industry, Innovation and Infrastructure, and SDG10: Reduced Inequality and others, and the training materials and workflows can support SDG4: Quality Education.

### 3.5 A call for long-term investment in community-led research infrastructures as drivers of data FAIRification and provision/democratization of access

Sustainability of tools and models developed within research projects, which have by nature a limited lifetime of funding, is not easy to achieve and needs to be considered from the start of every project. One suggestion that arises from the analysis performed herein is that part of the sustainability approach could include consideration, as part of the early design stage, of which SDG(s) the tool and or its results addresses either directly or indirectly, as a basis then for considering how best to ensure accessibility and impact, including *via* emerging publishers platforms for SDG tools, as well as (for more established models, *via* the EU MIDAS (**https://ec.europa.eu/knowledge4policy/modelling/topic/corporate-modelling-inventory-knowledge-management_en**) (the Modelling Inventory and Knowledge Management System of the European Commission), which is currently run and maintained at the Joint Research Centre of the European Commission (JRC-EC), and which has mapped the EU institutionally implemented models against the SDGs.

One requirement essential for being able to support the high-level goals of the SDGs is that the projects achieve their full impact, which will be the case only after the end of the project and, thus, depends on exploitation and reaching sustainability of the results and solutions provided by the project. Compiling examples of successful and failed sustainability efforts and experiences was identified as a first step to guide ourselves and other projects.

As normal practice for all EU projects, the tools/services offered by the NanoCommons Knowledge Infrastructure are developed and owned by NanoCommons project partners. They encompass multiple technologies and multiple programming languages. Establishing a single standard approach for software development would be impractical for the project partners and the wider community since it would be very limiting, not be able to keep up with the developments distributed across many organisations and projects globally, and incompatible, at least in parts, to most existing and emerging tools and platforms. Nevertheless, interoperability is essential for avoiding constantly reinventing the wheel and keeping pace with the need for new advanced materials. Integration of these numerous and diverse services into an interoperable environment requires some form of standardisation. Instead of standardising the underlying technologies, one possible solution is using a service-based architecture and standardising interfacing and data exchange as well as deployment of tools and services by using containerization. Delivery of software components in the form of containers gives the tool developer the freedom to select his/her preferred means for implementing the services (free choice of programming language/implementation in multiple environments *etc.*) with limitations only on the provided application programming interface (API). NanoCommons did not propose a one-size-fits all solution, but rather designed itself to be adaptive and responsive to the breadth of semantics, APIs and communication approaches already available in the nanoinformatics and chemoinformatics fields. In NanoCommons, this was achieved by defining and constantly refining guidelines for the development and adaptation of exchange formats, metadata standards and APIs, through which the data transfer, parametrization and execution of the services are performed, and which allowed for the combination of the services into workflows or the development of graphical user interfaces on top of the services to provide user-friendly access to the tools or models. However, such a flexible approach only works if maintenance and further developments can be guaranteed in the long run, through continued investment.

An example of the need for ongoing infrastructure investment is the Nanosafety Data Interface (**https://search.data.enanomapper.net/**) data management concept,[21] which started its development in the eNanoMapper project, continued to be extended by project-specific databases built on different database systems (*e.g.*, RiskGONE (**https://cordis.europa.eu/project/id/814425**), NanoFASE (**https://cordis.europa.eu/project/id/646002**)), and finally came together by the semantic integration model developed within, and provided by, the NanoCommons KnowledgeBase (**https://ssl.biomax.de/nanocommons/cgi/login_bioxm_portal.cgi**)[22] which indexes metadata from many of these databases and provides a common access interface. While the semantic integration framework of the NanoCommons KnowledgeBase was developed from private funding its extension towards nano-specific applications and its integration with the eNanoMapper/AMBIT (**https://search.data.enanomapper.net/datamodel/**) framework of individual data warehouses required funding from several nano-specific projects such as nanoMILE (**http://nanomile.eu-vri.eu/**) and NanoCommons. Maintenance of the NanoCommons KnowledgeBase infrastructure can be continued on low resource requirements from public funding, any data management support service, such as the data shepherding services, or further development of the data schema and services will require new public project funding as long as there is no commercial interest in these services. This is a symptomatic dilemma for sustainable data management tools for public data. Firstly, they require service and further development in addition to maintenance. Secondly, it takes an extremely long time to move new infrastructures such as nanoinformatics into long-term infrastructure funding schemes. Just as an example, molecular biology databases and bioinformatics tools were only made sustainable by large institutions such as the European Molecular Biology Laboratory and the National Center for Biotechnology Information taking them under their umbrella. Only decades later did actual infrastructure funding, for example the European Bioinformatics Institute (EMBL-EBI (**http://www.ebi.ac.uk/**)), arose to take over their management and maintenance. Quality evaluation of human and environmental toxicity studies performed with nanomaterials – the GUIDEnano approach.

An ongoing sustainability challenge is the GUIDEnano tool (**https://tool.guidenano.eu/**)[23] for risk assessment of nanomaterials across their life cycle, that began its development as a project internal tool, was publicly released and attracted interest from many projects to be the basis for further developments. Although the GUIDEnano project ended in 2017, the tool developers and the coordinator managed to further develop the tool and ensure its onward development *via* inclusion in subsequent European projects (caLIBRAte (**https://cordis.europa.eu/project/id/686239**), NanoCommons (**http://www.nanocommons.eu/**), GRACIOUS (**https://cordis.europa.eu/project/id/760840**), SAbyNA (**https://cordis.europa.eu/project/id/862419**)), and with some internal resources. NanoCommons, as one of the projects supporting the onward development of the tool, intended to offer access to an open-source version of the GUIDEnano tool to any user. However, significant intellectual property challenges and software access issues were thrown-up by the efforts to integrate GUIDEnano into the NanoCommons integrated modelling platform, which required development of work-around solutions by NanoCommons partners including establishment of a dedicated NanoCommons GUIDEnano version, with a limited set of exposure scenarios, which does not include recent developments due to the multi-project ownership model (SAbyNA, GRACIOUS), NanoCommons supported the development of training materials, a helpdesk for users and bug resolution support to ensure user friendly access. A key lesson from this scenario is the need for clear management of intellectual property rights such that open-source code versions of tools are provided to facilitate community development and prevent onward development, adaptation and reuse being restricted due to intellectual property constraints.

We recognise and commend the significant investments in the European Open Science Cloud (**https://eosc-portal.eu/**) (EOSC) to develop a Web of FAIR Data and services for science in Europe upon which a wide range of value-added services can be built, but identify a gap between such large scale highly technical top-down initiatives and the community-driven bottom-up approaches such as those such as NanoCommons, a "starting community" that has yet to reach the critical mass needed to fully inter-operate with EOSC. We thus call for additional and follow-on funding for such bottom-up and bridging funding to help scale-up these communities and bridge the gaps. Such follow-on funding could facilitate the establishment of natural hubs or non-profit organisations dedicated to the mission of the SDGs, representing the community and the greater good, rather than being profit oriented, with the goal of democratising access to tools and models. Such an approach would also address the concerns of users/project developers about handing their intellectual property to another company/SME.

### 3.6 Summary of the role of FAIR nanosafety data and nanoinformatics as a means to address the SDGs

As noted earlier in this paper, the United Nations Task Force on Science, Technology and Innovation evaluated the potential of nanotechnology for sustainable development based on the UN Millennium Development Goals.[24] Table 1 shows part of the original mapping of the 10 major application areas for nanotechnologies,[25] and provides an extension of this, based on research performed herein, to map these areas of nanotechnology, nanoinformatics and FAIR nanosafety data to the SDGs. The table demonstrates explicitly the role of easily accessible FAIR nanomaterials environmental health and safety (nanoEHS) data and nanoinformatics tools as drivers of progress towards the SDGs, focussing on just some of the ways ontologies, predictive models for cytotoxicity, exposure, biodistribution (PBPK models), drug repurposing, allergen exposure, risk assessment and more can support progress in achieving all 17 of the SDGs.

Based on the analysis presented in Table 1, and the survey feedback from the provision of access to nanoEHS data and *in silico* models, it is clear that FAIRification of nanomaterials data and democratisation of access to nanoinformatics models and data will facilitate progress in all 17 SDGs. While all 10 areas identified in the 2005 mapping are still relevant, there is considerable overlap in their mapping to the SGDs as shown in Table 1, and this we have merged these into 5 overarching areas where FAIR nanosafety data and nanoinformatics can drive the SDGs as shown in Fig. 6: in nano-enabled sustainable agriculture and aquaculture *e.g.*, ref. 28 and 29 which also covered vector and pest detection and control, in materials for energy capture *e.g.*, 30, in nanomedicine which covers diagnosis, health monitoring and drug delivery systems *e.g.*, ref. 25 and 31, in pollution remediation which includes air pollution and remediation,[32] and in terms of wider social implications and impacts. Several SDGs fall under more than one of these broad categories, highlighting the interdependence between the SDGs also. We note also that the recent Roadmap from the Advanced Materials Initiative 2030 (AMI2030 (**https://www.ami2030.eu/roadmap/**)) prioritises advanced materials for use in 9 categories: Health Care, Sustainable Construction, Sustainable Transport, Home & Personal Care, Sustainable Packaging, Sustainable Agriculture, Sustainable Textiles, Electronics Appliances and New Energies.

A key aspect of NanoCommons' effort has been to reduce the barriers to the use of nanoinformatics approaches by developing and providing user-friendly graphical user interfaces for complex and advanced models, such that they can be utilised by those who are not trained or proficient in coding and programming. Such democratisation of access to nanoinformatics will play an important role in facilitating the uptake and use of *in silico* approaches for nanoEHS in developing countries, and indeed the more agile regulatory environments in these countries may even facilitate more rapid adoption of so-called New and Emerging methods (new approach methodologies, NAMs) as *in silico* tools become more available and user-friendly. But to achieve this, several collective advances are needed, including (i) integration of *in silico* methods and NAMs into the OECD's Mutual Acceptance of Data (MAD) process and (ii) agreement on governance approaches related to the democratisation of artificial intelligence (AI) approaches more generally, including in the context of medicine and healthcare. Here we are focussed on democratising access to AI tools and datasets *via* open or easy access to code libraries, developer tools, and data sets, whereby access to these tools allows materials experts/regulators without software development skills to contribute to wider use of AI in nanosafety assessment and safe by design of materials. However, the use of the term democratisation of AI is also positioned in a wider context of different understandings of the role of AI as a transformative agent that can democratise medicine and healthcare. Rubeis *et al.* (2022) conclude that democratisation in the context of AI in healthcare requires defining and envisioning a set of social goods (benefits) as well as deliberative processes and modes of participation to ensure that those affected by AI in healthcare have a say in its development and use.[33] Similar considerations apply for nanoEHS and nanoinformatics, especially in the context of their use in driving progress towards the SDGs.

*In silico* tools have a bright future in toxicology. More specifically, they assist a critical assessment of our toolbox, and they help to combine various approaches in more intelligent ways than a battery of tests. At the same time, their use value is determined by the underlying science as "no model can overcome a series of bad assumptions".[34] More than 10 years ago it was noted that "the *in silico*/QSAR field is facing more resistance in traditional toxicology than it deserves, though some is appropriate and necessary" and that it has been suggested that this can arise both due to inappropriate use of QSAR for chemicals that elicit different mechanisms and from the intentional and unintentional over-selling of the predictive capabilities of QSAR.[35] A key feature of data sharing in chemicals (and materials) safety assessment is the Mutual Acceptance of Data (MAD), a multilateral agreement where national approaches to regulation of nonclinical safety studies are harmonised so that data generated in an OECD member country can be accepted in other member states provided the test methods are in acquiescence with the OECD Principles of Good Laboratory Practice (GLP) and the OECD Test guidelines.[36] The MAD system aims to avoid contradictory or duplicative national requirements, reduce non-tariff barriers to trade and offers a common platform for cooperation amongst national

 

Table 1 Mapping of the NanoCommons TA projects on FAIRification of nanoEHS data and nanoinformatics tools to the 10 grand challenges to be addressed by nanotechnologies as identified in ref. 25, mapped to the SDGs. While the models and data management workflows developed in NanoCommons focussed primarily on exposure, toxicity and risk aspects of the nanoscale materials, they can be loosely allocated to the 10 different application areas identified in the original mapping as shown here, and to clusters of the SDGs. Note that these are examples only. The full list of TA project titles (and the TA provider and user organisations) is provided in ESI 2. A searchable version of the table is presented in the ESI as Supporting Material 4

| Applications of Nanotechnolog y | NanoCommons TA project: role of FAIR nanoEHS data and/or nanoinformatics in supporting the SDGs | How nanoinformatics data and/or tools directly or indirectly support the SDGs (not a 1:1 mapping but rather an overview for each of the goals) |
|---|---|---|
| Energy storage, production, and conversion | NC01 - Ontologies for nanodescriptors generated by molecular modelling<br>• Inorganic NMs such as metal oxides are key to energy storage and capture devices.<br>• Ontology terms covered materials descriptors as well as materials application areas and meta-models that bridge across scales.<br>• Documentation of the interlinkages between materials models *via* MODA templates to link models for materials properties with models for materials functionality (*e.g.*, energy capture).<br><br>NC12 - Cremations, urns and mobility. Ancient population dynamics in Belgium, XRD analysis and crystallographic modelling<br>• Mapping historical cremated bones: use of spectral data to understand historical burial practices<br>• Links to social and cultural norms in different countries related to burial practices and energy demands associated with these.<br>• Ethics of data-re-use and data governance. | SDG7: Affordable & clean energy<br>- The *in silico* data enrichment tools can help to identify NMs features optimised for energy capture/storage, that support reduced greenhouse gas emissions (*e.g.*, through more complete combustion) and/or for use in construction materials, driving sustainable and green innovation.<br>- Full documentation of models (*via* MODA) is a critical step in driving uptake/market acceptance of the tools (i.e., standardisation) and the detailed tutorials and user guidance are key steps in democratising access for global south to models and datasets.<br><br>SDG4: Quality education<br>- Extensive training materials have been developed to accompany all NanoCommons models, as part of the efforts to democratise access to advanced approaches. Additional materials for use in schools and universities are being developed also, enabled by the fact that all NanoCommons models have free user-friendly graphical user interfaces, requiring only an internet connection rather than specific software licences or other potentially prohibitive resources. |
| Agricultural productivity enhancement | NC3 - Data curation & harmonization: increasing fairness scores and availability of data generated under EU projects (NanoFASE, NanoFARM)<br>• Agricultural productivity is dependent on soil quality including bacterial richness and earthworm bioturbation to aerate.<br>• Datasets covered impacts of Ag NMs on earthworms and soil and water mesocosms.<br>• Development of instance maps to structure the data and associated metadata to facilitate re-use of the data, including for development of predictive models.<br>• Implementation of new ontology terms and mappings for NMs transformation processes such as sulfidation which determine NMs persistence & ecosystem-level impacts such as soil quality. | SDG15: Life on land<br>- The impact of intensive agriculture on soil quality has been dramatic with many soils having < 10 years of productivity remaining, which has consequences for food security. The development of streamlined data curation processes for soil quality data, and earthworm/bioturbator data (*e.g.* NanoFASE, NanoFARM, & data regarding the impacts of nanomaterials on soil microbial composition and functioning and earthworm behaviour), provides a strong basis for further harvesting relevant datasets, both to facilitate the development of models to predict impacts of treatments on soil health and thus productivity (and health) and to develop relevant policy interventions to support and drive initiatives to improve soil health, while maintaining productivity and sustaining livelihoods in developing, agriculture-based economies. |
| | NC07 - Using image descriptors to predict nanomaterials zeta potential<br>• Development of agrochemicals: zeta potential can be used to predict the stability and dispersibility of the particles in the formulation. This can affect efficacy and environmental impact of agrochemicals. By manipulating zeta potential of particles, it may be possible to enhance performance and reduce the environmental impact of agrochemicals.<br>• Zeta potential of soil particles can affect the ability of the soil to retain nutrients and water, as well as the movement of pollutants. Predicting the zeta potential of soil particles can help to optimise management practices such as irrigation, nutrient application, and soil remediation.<br>• Climate change, gender inequality and responsible production all converge in managing soil quality. | SDG12: Responsible consumption & production<br>- The TA project with Brazil supported the introduction of FAIR data management approaches to the national centre for nanotechnologies, from which it also rolled into national standardisation activities on nanotechnologies including the MCTI-INMETRO-SisNANO programme. for Certification of Nanoproducts). Early access to the state of the art in nanosafety data management and FAIR data, and the expertise to support its implementation in the Brazilian context has been extremely beneficial, as has the experience of understanding how to adapt technologies and solutions for the local context integrating local knowledge. |
| Vector and pest detection and control | NC10 - Structural alterations of allergen upon nanoparticle binding & NC17 - Mixture (nano)toxicity in the *Daphnia magna* Model<br>• Both of these TAs considered the interactions of NMs with co-pollutants, and the role of the biomolecule corona directly (allergens) and indirectly (binding co-pollutants and changing their bioavailability) on the activity/toxicity.<br>• Such approaches/models can also be applied to assessment of the role of NMs as vectors for viruses or bacteria, or to design NMs-based sensors for key proteins or environmental DNA (so-called eDNA) for example.<br>• Models for mixture assessment are critical to understand the potential risks of NMs activating as vectors for transport of other entities, including bacteria. Indeed, air pollution particle levels were found to correlate with Covid-19 infectiousness.<br><br>NC16 - Data capturing, storage and management of high quality, curated and harmonized data generated under the ASINA project while increasing fairness scores<br>• ASINA were one of the first projects to implement the NanoCommons data shepherding approaches, applying them to management of case studies.<br>• A case study explored anti-microbial and anti-biofilm coatings for | SDG16: Peace and Justice through strong institutions<br>- Nanomaterials safety is an example of a community of practitioners who tried to preempt problems such as unsafe nano-enabled products reaching the market, and public opinion turning against the technology as a whole (as was the case what genetically modified organisms in the EU), through application of governance approaches early. This also involved ongoing engagement with all relevant actors including regulatory agencies and industry to ensure that regulators were aware of scientific progress. That said, there is still room for further improvement - for example, research data is still difficult to integrate into regulatory risk assessments despite the fact that research is usually a decade ahead in understanding than regulation is. Data and model documentation, including rich metadata, is a key aspect to improving the re-use of research data and models in governance, regulatory risk assessment. NanoCommons efforts, including in elucidating the need for a dedicate role of “data shepherd” to support this transition, is key. |

Table 1 *Contd.*

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| | textiles, and established reporting guidance and data templates to facilitate researchers and the industrial community to disclose appropriate functionality data *via* the FAIR principles.<br>• Datasets were made increasingly FAIR through data shepherding, and SOPs for data management were implemented (19). | |
| Water treatment and remediation | NC17 - Mixture (nano)toxicity in *Daphnia magna*l - Supporting FAIR data practices in Brazil<br>• Project involved knowledge transfer to support establishment of FAIR data management practices in national Brazilian nanotech labs, and then further roll-out to other laboratories in Brazil.<br>• Implemented Electronic Laboratory Notebook, Instance Maps and data integration in KnowledgeBase for a set of studies exploring the impact of graphene (and its adsorbed biomolecule corona) as a mediator of the toxicity of heavy metal pollution in aquatic systems (27).<br>• Nanomaterials' capacity to absorb co-pollutants, and the impacts of adsorption to NMs for the toxicity of co-pollutants was explored & all data/metadata made FAIR.<br>• Use of the "Instance map" tool allows understanding of impact of the environment and points where the NMs may transform and thus behave differently. NanoCommons has proposed instance maps as a tool for quality assurance and for integration and harmonisation of datasets.<br>• Extensive training materials developed to support wider roll-out in Brazil.<br><br>NC29 - Data integration for online analysis of production parameters on material properties & quality<br>• Continuous or in-line characterisation of materials properties and quality raises additional data management challenges, related to the quantity of data and the need to understand what is relevant for internal Quality control versus what might have intrinsic value for broader nanoEHS assessment and modelling, for example.<br>• Data shepherding approaches will maximise the transfer of knowledge and data. | SDG6: Clean water & sanitation<br>- There were an estimated 13.7 million infection-related deaths in 2019. Malaria alone kills half a million annually, despite progress in impregnating nets with pesticides targeting mosquitos. Textile hygiene and infection control measures have become increasingly important in recent years due to the growing concerns about textiles as fomites (inanimate objects that can carry and spread disease and infectious agents) in healthcare settings (26). NMs composed of silver and copper have antimicrobial properties and are being embedded into textiles for a range of essential (*e.g.*, wound and burn dressings) and less-essential (*e.g.*, odour reduction socks and sports cloths) applications. However, concerns exist that the NMs are quickly washed away thus limiting long-term effectiveness and thus applications of safe-by-design to ensure longevity of effect are essential, but not inadvertently introducing new problems related to over-persistence in the environment and/or at end of life. Sharing of data and experiences, such as *via* the ASINA case study on antimicrobial textiles, are thus essential to support transfer of knowledge and enable new innovations to support global health and wellbeing and to ensure that the advances are not limited to global north countries, given that the majority of infectious-disease deaths occur in the global south.<br><br>SDG14: Life below water<br>- Daphnia magna are an important indicator species for water pollution globally, with 2 tests included in the OECD Mutual Acceptance of Data (acute and chronic (reproductive) toxicity to daphnia) framework, meaning that data from one country performed in accordance with the agreed Test Guidelines is accepted for regulatory purposes in another country. Thus, sharing of data from standard (OECD) test guidelines is critical to support regulations globally, and to enable nanomaterials approved in one jurisdiction to be approved elsewhere on the basis of the same datasets. |
| Disease diagnosis and screening/Health monitoring | NC15 - Assist the Diamond SARS-CoV-2 Mpro fragment screening program in selecting compounds for further analysis based on predictive metabolism and toxicology<br>• Covid rapid response demonstrating potential of re-use of both data & modelling tools to address urgent healthcare issues.<br>• Reduction of inequality (of access and knowledge) through collaboration, knowledge and informatics tool and expertise sharing.<br>• Workflows for model integration and screening of existing drugs fragments.<br><br>NC33 - Bioinformatics analysis of transcriptomics $TiO_2$ dataset (from inhalation exposure studies in the context of the SmartNanoTox project)<br>• Biomarkers of disease are typically identified from omics data, and identification of molecular initiating events leading to Adverse Outcomes is expected to accelerate understanding of pollution-related disease mechanisms.<br>• Existing data processing workflows were applied (re-use of tools and approaches) to datasets and the resulting processed data was FAIRified;<br>• Potential to reduce gender inequality in medicine through considering impact of sex on model results, *e.g.* modelling male vs female sera.<br><br>NC4 - Computational analysis of mesothelioma expression profiling data with Enalos Chem/Nano Informatics Tools: potential to support disease diagnosis and screening by identifying significant genes that can discriminate between pathological and healthy samples.<br>• The developed QSAR model can predict the long-term toxicity of fibre nanomaterials based on gene expression signatures, which can aid in screening and diagnosis of diseases related to nanomaterial exposure.<br>• The standardization and normalization of expression profiling data can improve data comparability across studies and facilitate the identification of biomarkers of disease.<br>• The Enalos KNIME nodes used in the workflow can enable the integration and analysis of diverse data types, such as chemical properties and toxicological endpoints, which can further enhance disease diagnosis and screening. | SDG10: Reduced inequalities<br>- Agriculture is one of the major polluters due to excessive use of nitrogen-based fertilisers ($N_2O$ is a greenhouse gas), much of which runoff into water bodies, and over-reliance on pesticides. NanoCommons datasets and models enable tuning of nanomaterials properties and prediction of their fate and behaviour and/or toxicity to soil and water environments, providing a basis for design of nano-enabled agrichemicals that are less harmful to soil, air and water whilst delivering the pest control needed.<br>- Democratisation of access to data and models, through provision of user-friendly graphical interfaces with no need for coding, and the underpinning datasets as easily downloaded formatted sheets, is a major step towards reducing inequalities in terms of knowledge and access across boundaries and scales. Nanoinformatics and FAIR nanomaterials and nanosafety data and models provide an initial understanding of the potential hazards and risks of nanoscale materials and a basis from which to tailor existing models to the local needs and conditions of communities in the global south. Use of open access tools and software means that the tools can be easily tailored to local needs by software developers, and where the relevant expertise is not available the contact details for collaborative re-development of models for specific needs are provided with all NanoCommons models and tools.<br>- A key finding from the Covid-related TA project was that once models have been developed it is relatively straightforward and quick to re-purpose them for other applications, and that datasets collected and curated for one purpose can be leveraged and mined to support other, often quite different, research and policy questions. This was a strong argument for FAIR data practices.<br>- Many of the approaches developed in NanoCommons, especially around best practice in making research data and nanoinformatics software FAIR (Findable, Accessible, Interoperable and Reusable) have been further developed in other projects, including NanoSolveIT, CompSafeNano and MACRAMÉ, and are being systematised and documented as how-to guides *via* the WorldFAIR project, which aims to support global best practice within and between domains to support achievement of the SDG.<br><br>SDG5: Gender equality<br>- Despite progress in understanding of differences in disease susceptibility |

 

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| | • The developed model's read-across capabilities allow prediction of toxicity of similar nanomaterials based on their Euclidean distances, accelerating identification of potential disease risks associated with new or under-studied NMs.<br><br>NC20 - Predictive toxicity assessment of semiconductor quantum dots that are used as fluorescence probes – adverse effects on the human lung epithelial carcinoma cell line A549 ("QD-cytotox")<br>• Nanomedicine and nano-based sensors are increasingly being utilised in health monitoring and control, and were critical to both the testing for, and vaccination against, Covid-19.<br>• Ensuring the safety of nanomedicines and nanosensors is critical: predictive models such as Quantitative Structure-Activity Relationship (QSAR) models to predict the health implications for nanomedicines are critical.<br>Provision of user-friendly interfaces and detailed training materials, modelling-ready datasets, fully documented models and underpinning datasets, and best practice for these steps are key outcomes from NanoCommons relevant to multiple SDGs. | between sexes (*e.g.*, women have double the risk for Alzhemier's disease than men) and differences in responses to drugs and medications, there are still major disparities in provision of tailored healthcare to women. The NanoCommons approaches, including biomarker discovery, biomolecule binding assays, determination of the Molecular Initiating Events leading to Adverse Outcomes and the associated Adverse Outcome Pathways (AOPs) can facilitate progress towards sex-considerations in design and testing of medicines, including nanomedicines, and through consideration of hormone and sex-specific interactions. |
| Drug delivery systems | NC25 - Stochastic optimisation for grouping nanoPBPK model parameters and estimating their values: New methodology and service development<br>• nanoPBPK models are essential to predict the biodistribution of nanomedicines for example, to ensure they reach the target site and remain there for the required duration.<br>• Within NanoCommons the first compilation of nanoPBPK models was developed and these were made available for re-use and further development/parameterisation (to cover additional NMs for example) and bespoke models were also developed to fit users' needs.<br>• Providing user-friendly graphical interfaces and simplifying the processes for inputting parameters reduces training barriers and democratises access to models, predictions and progress.<br><br>NC23 - PBPK model on 99m-Technetium labelled carbon nanoparticles inhaled by humans: Implementation in R and integration into NanoCommons modelling toolbox.<br>• The service provided here was re-coding of existing models into the mode accessible R programme, which also facilitated integration with other models into a modelling workflow.<br>• Providing user-friendly graphical interfaces reduced the need for coding skills and thus reduces barriers to access/democratizes access.<br>• Integration of the re-coded models into the NanoCommons modelling toolbox ensures stability of access and sustainability. | SDG1: No poverty<br>- The PBPK, QSAR and other predictive models developed in NanoCommons can be re-parameterised for different organisms, and re-purposed for design of anti-viral agents, such as anti-fungals to reduce pest impacts on crop production and thus increase food security and small-farm profitability through reduced crop losses.<br>- The democratisation of data and modelling tools for nanosafety assessment and Safe and Sustainable by design nanomaterials development, as pioneered by NanoCommons, is an important step towards levelling the playing field and thus reducing poverty through access to innovation, education and ability to tailor approaches to the local conditions.<br><br>SDG9: Industry, innovation & infrastructure<br>- Start-ups and community innovation clusters rarely have access to specialist knowledge and computational expertise. Democratising access to nanoEHS tools and datasets enables responsible choices whilst supporting local innovation potential. The breadth of application areas for data-driven modelling approaches, and safe-by-design materials are endless, and sharing of knowledge and cross-fertilisation of normally disparate industry sectors offers enormous potential for innovation.<br>Infrastructure projects, like NanoCommons offer a platform for connecting ideas and people, through provision of tools, networking, training opportunities and expertise to support implementation and operationalisation. |
| Air pollution and remediation | NC16 - Data capturing, storage and management of high quality, curated and harmonized data generated under the ASINA project while increasing fairness scores<br>• Field Exposure Monitoring (FEM) campaigns produce a significant amount of data that are valuable for emissions, exposure and risk assessment, as well as providing insights into the factors affecting process emissions, exposure levels and risks.<br>• Using the data shepherding approach, the TA provided an annotated template for capturing FEM data, and increased their interoperability, and re-usability for exposure and risk assessment (18).<br>• Applicability for assessment of occupational exposure during production to provide safer workspaces and protect health.<br><br>NC10 - Structural alterations of allergen upon nanoparticle binding<br>• Allergens are increasingly prevalent in the environment, including pollen.<br>• Through combination of experimental and computational data, new insights into interactions of allergens with nanomaterials were gained, and increasingly predictive models were generated (16).<br>• Increased utility of the models for predicting protein (allergen) binding to nanomaterials and fully documented models to increase regulatory trust as models become increasingly validated. | SDG3: Good health and well-being<br>- Collectively the projects that developed models for assessing/predicting impacts of nanoscale entities on living systems, whether intentionally destructive interactions (killing the virus) or unintentional impacts of materials designed for diagnostic or therapeutic effects, provide a strong starting point and best practice for development of additional models and understanding of health and well-being. Data and model sharing are critical to maximise translation of knowledge and to safe re-purposing of tools and approaches to new challenges, where existing approaches can be deployed rapidly to tackle new disease-related questions.<br><br>SDG17: Partnerships for the Goals<br>- NanoCommons's main objective was to build a community of practice, and the underpinning support to drive change in research culture, such that the management and sharing of data was moved to the point of data collection, rather than being something performed under duress at the end of the project, to fulfil funder mandates. The TA activities presented herein were a clear example of the benefits of partnership, whereby one party had a problem or research question to be addressed and the other had a potential solution that could be applied, tailored and tweaked to meet the research need. Scaling this up to addressing global challenges, demonstrates the need for actors who can connect needs and solutions, and an essential part of this is open and FAIR data and models, where re-use and derivation conditions are clear and foster growth and innovation. |
| Construction | NC21 - Implementation and validation of the FAIR principle for data produced in SAbyNA project to ensure that high quality data is flowing into data repository | SDG11 - Sustainable cities and communities<br>- The mixture toxicity datasets and models, developed in NanoCommons or elsewhere, as represented by the *Daphnia magna* model, is an important step |

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| | • As a case study within SAbyNA, 3D printing and paint are used, where exposure to nanomaterials is possible. Assessment of approaches to reduce exposure through application of SbD approaches.<br>• *Via* the TA, extensive knowledge building on FAIR data management workflows was provided.<br>• Data are being incorporated into the NanoCommons KnowledgeBase (data warehouse, (22)) to facilitate data re-use for modelling for occupational and consumer risk assessment.<br><br>NC04 - Computational analysis of mesothelioma expression profiling data with Enalos Informatics Tool<br>• Occupational exposure is considered during construction, and especially during demolition of ulcer buildings where asbestos or other known toxic particles may be present.<br>• Open access modelling tool developed for analysis of mesothelioma expression profiling data to provide low-cost predictions of hazard.<br>• User-friendly graphical interfaces that reduce the need for programming skills are critical to democratise machine learning/AI. | towards understanding the combined effects of pollutants in the environment, including the potential for nanomaterials to mitigate the impacts of other pollutants. Such data and models can be used as a basis for prioritisation of chemicals or for identification of pollution hot-spots for remediation, for example.<br>- By understanding interactions between chemicals, and the combined effects of chemical mixtures on model organisms, approaches such as Safe-by-design can be applied as part of responsible innovation, to support safety and more sustainable chemicals and materials, while maintaining functionality. Making such data and tools available freely, as part of efforts to democratise access, supports industry and innovation. |

authorities. It has been estimated to save industry and governments around €309 million every year. In this vein, a recent impact analysis study on the Indian National GLP Program in 2019–2020 assessed the impact of the first decade of India having full-adherent status to MAD in the OECD[36] and found that by 2019–2020, Indian test facilities had conducted more than 60 000 nonclinical safety studies, valued at INR 7800 crores (USD 1.3 billion), representing a major step toward self-reliance in the development of New Chemical Entities. To date, *in silico* approaches to toxicology have not been widely accepted in regulation, and a significant roadblock to this is that there is no equivalent of GLP for modelling and simulation. To overcome this gap, the In Silico World (**https://insilico.world/community/good-simulation-practice/**) community of practice is hosting the consensus process to develop the so-called Good Simulation Practice. The Task Force defines *In Silico* Trials as the use of computer simulation to assess the safety and/or efficacy of new health care, whether medical devices or medicinal products, and this could also be extended to safety assessment of chemicals and materials as well as MAD in due course. The impact for the SDGs, especially SDG3 (Good health and wellbeing for all), would be significant.

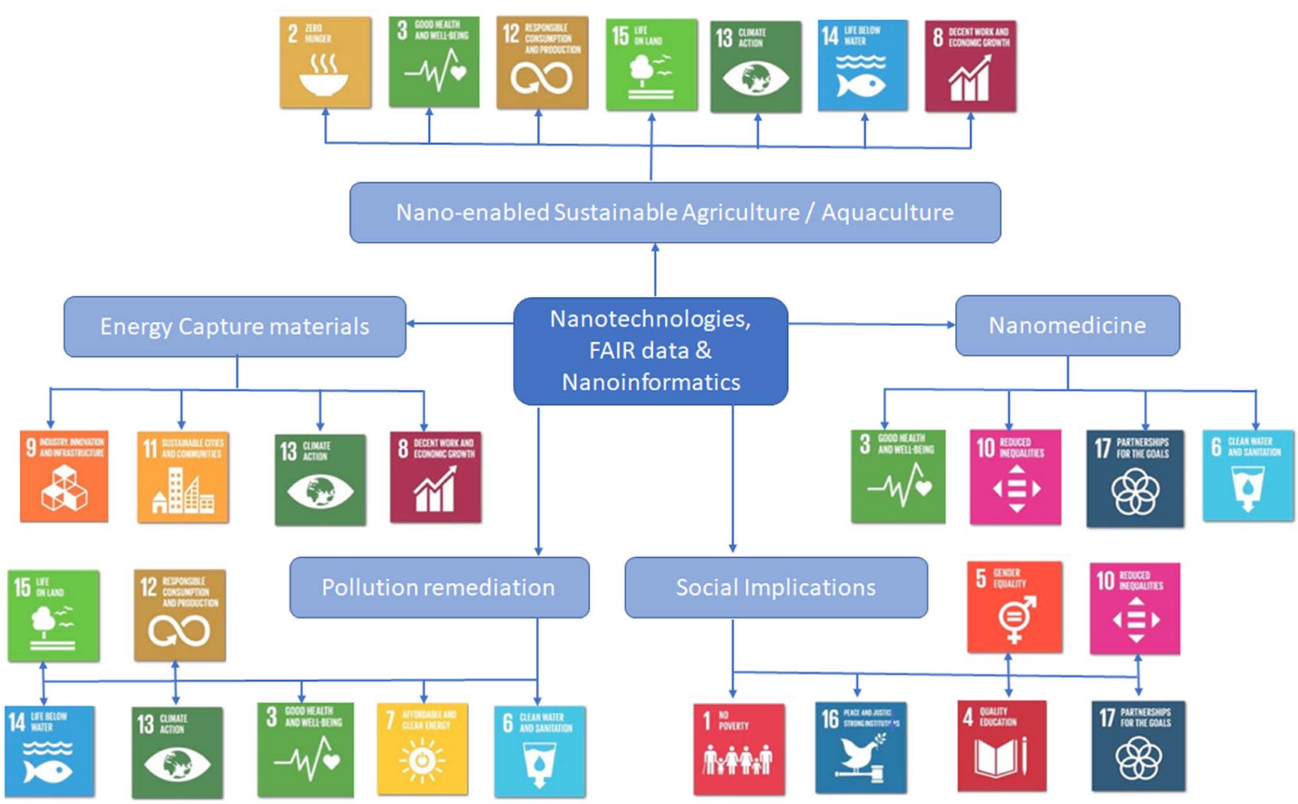


Fig. 6 Mapping of the main application areas of nanomaterials and FAIR nanoSafety data and informatics tools to the SDGs.

As part of the social implications pillar in Fig. 6, we note especially the need for researchers and practitioners to ensure that interventions are well thought-through and embedded in local practice. An important lesson from past adaptation interventions is that within current adaptation *cum* development paradigms, inequitable terms of engagement with 'vulnerable' populations are reproduced and the multi-scalar processes driving vulnerability remain largely ignored. In particular, instead of designing projects to change the practices of marginalised populations, learning processes within organisations and with marginalised populations must be placed at the centre of adaptation objectives.[37] Here, in addition to the FAIR principles, the CARE Principles (of Collective benefit, Authority to control, Responsibility, and Ethics, and their respective sub-principles) for Indigenous Data Governance should also be applied, as these address concerns related to people and the purpose of data.[7] The CARE Principles detail that the use of Indigenous data should result in tangible benefits for Indigenous collectives through inclusive development and innovation, improved governance and citizen engagement, and result in equitable outcomes.[7]

# 4 Conclusion

As a research infrastructure focussed on building a community of practice around digital and *in silico* approaches for assessment of the safety of nanoscale materials, including the implementation of best practice in data management across the data life cycle, and increased FAIRness of nanoEHS data, an assessment of the effectiveness of our services and tools was a critical component. In parallel with the transition throughout the period of Horizon 2020 from safe-by-design materials to safe-and-sustainable-by-design materials, the NanoCommons consortium focussed increasingly on the sustainability aspects of our work, including an assessment of the ability of our research infrastructure to support the achievement of the UN SDGs.

In total 12 SDGs were identified as relevant from the evaluation of the NanoCommons tools and services as provided *via* the "access" programme. Further analysis as part of the preparation of our sustainability deliverables and our demonstration case studies led to the recognition that nanotechnology coupled with FAIR nanosafety data and user-friendly access to advanced modelling tools without the need for programming skills, will support progress towards all 17 SDGs, with the SDGs grouped around 5 key nano-enabling areas: nano-enabled sustainable agriculture and aquaculture, materials for energy capture, nanomedicine, pollution remediation and wider social implications and impacts. Democratisation of access to technology, AI and *in silico* materials safety tools and data will facilitate the transition to safe and sustainable nanotechnology-enabled solutions addressing the breadth of the SDGs.

Key challenges remain though, including the need to sustain and fund research infrastructures, the need to develop approaches to support uptake of nanoinformatics approaches into regulatory frameworks, such as through the Good Simulation Practice initiative, and development of a governance framework to advance democratisation of access to, and benefits from, *in silico* approaches and artificial intelligence for materials safety assessment. We are confident that the way forward for achievement of the SDGs is through a "commons" approach, in which cultural, natural or knowledge (in this case) resources are collectively owned and accessible to all members of a society. As highlighted by this paper, community ownership and collective responsibility is based on the provision of free to access services for FAIR data management and nanoinformatics tools. Training and awareness building remain a high priority to ensure that researchers understand the value of their research beyond their own immediate needs and include aspects for sustaining and strengthening the commons and the benefits resulting from it already from the design phase for new developments and investigations.

# Author contributions

Conceptualization: BA, TE, IL. Formal Analysis: BA, TE, JDO, IL. Funding acquisition: IL, TE, AA, HS, DM, SV, VL, GM, EW. Methodology: BA, SR, CW, IL. Project administration: LCG, IL, TE. Resources: AP, AA, GM, VL, MH, HS, IL, EW. Software: AA, VL, HS, Supervision: AF, SV, JDO, IL, Visualization: BA, GM, IL. Writing – original draft: BA, TE, LCG, NB, DM, IL. Writing – review & editing: All co-authors.

# Conflicts of interest

The authors declare that they have no competing interests with the content of the present study.

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