Marc Segers, Head of Product Innovation

LabConnect

Providing researchers with pathways to tools & facilities for nano/material science

FAIR Facilities and Instruments Workshop 3
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AIP Publishing

LAB CONNECT

Solves early-stage industry researcher planning and facility discovery problems by surfacing peer-reviewed articles, methods data, and linking needed instrumentation to accessible academic facilities

National Academies of Science report highlights facility discovery challenges

Instrumentation is difficult to locate

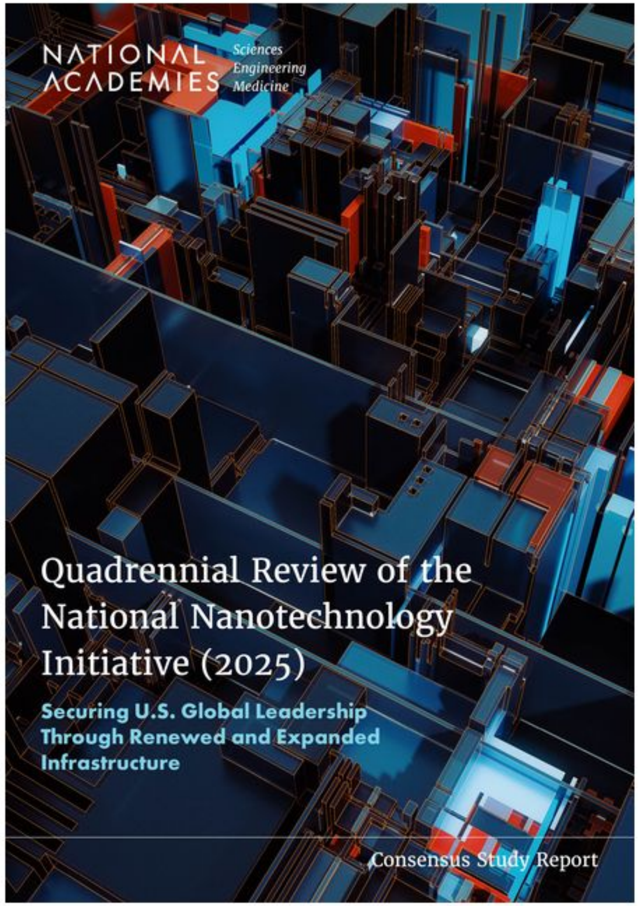
“There is no single source of information combining all of the capabilities of the nation’s nanotechnology infrastructure. At the federal level, potential users have to consult separate website listings . . . At the regional and local level, information can be hard to find.”

User discovery is primarily word-of-mouth

“The majority of users reported that they discovered information about the facility from conversations with other users. If professional networks are the primary vehicle for advertising the resources, then less well-resourced research institutions are at a disadvantage.”

A nation-wide index of nano facilities and their resources is needed

“**Recommendation 1.1:** In the coming year, the [NNCO] should conduct a census of accessible nanotechnology infrastructure sites (instruments, staff, facilities) and display findings . . . to enhance the visibility, availability, and impact of these assets.”



https://nap.nationalacademies.org/catalog/29063/quadrennial-review-of-the-national-nanotechnology-initiative-2025-securing-us

Insights from industry researcher interviews

"The same tool is $80/hr at Princeton, but $300/hr at Harvard - there is no price transparency… If there was a nationwide qualified system we could use, that would be a lifesaver - save a lot of time" - Wei Ting Chen, SNOChip

" Finding specialized tools takes a week - all through word of mouth...I would LOVE to see somebody process 10 GHz lithium niobate... if I could point to say 'this is where these people did it', that would drive industry forward" - Doug Bopp, Apex Atomics

"Wish there was a database that included capabilities of universities"
John Michaelk (Zebra Analytix)

"Absolutely think it would be helpful -- right now just rely on network and connections... it would be very helpful if it is there [in the tool]"
Vikas Nandwana, Coral Innovations

"I don't know what I don't know - need help understanding research pathways" - Benjamin Draper, Megadalton

"For a startup -- do a lot of things I don't have experience doing... there are fields I don't have connections / knowledge if there was a platform that gave me resources -- just the knowledge is most valuable"
Farid Kalhor, FemtoSense Labs

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Priorities & needs for companies by growth stage

Establishing 2 to 4 months	Experimenting 1 to 3 years	Expanding 3 to 6 years	Scaling 7 to 15 years
FTE: 1	FTE: 1 to 3	FTE: 2 to 10	FTE: 8 to 20+
Priority: Establishing company and finding place to do their work	**Priority:** Progressing their research with quick, impactful discoveries	**Priority:** Expanding operations with increasing specialization, refining products, and in-house capabilities	**Priority:** Managing multiple research projects with extensive planning and growing in-house capability
Facilities: Locating facilities by their existing network, word of mouth, internet searches to find low cost-accessible capabilities. Often use facilities from previous experience (univ)	**Facilities:** Using familiar facilities, may still search for outside facilities to supports specialized needs and supply chain flexibility	**Facilities:** Using trusted facilities but may require more discovery for specialized capabilities and small-scale fabrication. In-house capabilities may be developed to protect IP	**Facilities:** Running multiple projects with mix of industry, academic and in-house facilities. Lead times for planning may extend to 6mo., still need just-in-time access to facilities
Literature: Reading peer-reviewed articles to stay up to date with specific area of research for grant proposals	**Literature:** Consulting peer-reviewed articles for research planning and proposals	**Literature:** Consulting peer-reviewed articles for research planning and proposals – multiple team members need access	**Literature:** Consulting peer-reviewed articles for research planning and proposals across the R&D team.

Using articles to support research planning and facility discovery

On a weekly basis - industry researchers searching for how to progress their projects by:

- Reading relevant peer-reviewed articles
- Identifying common and novel techniques to answer their questions
- Extracting details like instruments, critical steps, experts to consult
- Locating facilities with the needed capabilities to use

What is your research question?

Gather peer-reviewed articles that address the question

Summarized research pathways: common techniques / novel techniques

Technique details including instruments, materials, experts for consultation

Facilities with instruments based on location, cost, and other preferences

Article data extraction and author verification

AIP Publishing POC showed a >80% accuracy rate with an automated AI data extraction process for article technique, material, and instrument data. Authors then verified data and provided facility references.

RhB degradation under simulated solar irradiation. This approach can provide useful information about EPs reaction pathways at the photocatalyst surface that drive the release of degradation products in the solution. This approach is of general interest, as it allows to investigate the initial stages of the degradation kinetics of any organic pollutant by following the evolution of several intermediate products at the photocatalyst surface simultaneously. Such information can be crucial for a proper tailoring of the modification of the photocatalyst aimed at the improvement of its performances, and it can be relevant, at least in principle, from the environmental point of view, since it can detect the formation, even in tiny traces, of harmful degradation by-products.

II. EXPERIMENT

A. TiO_2 films preparation

Absolute ethanol, phosphorus (V) oxychloride ($POCl_3$), and hydrated zirconyl chloride ($ZrOCl_2 \cdot H_2O$) were all purchased from Sigma-Aldrich and used as supplied. The water used in the experiments was of MilliQ quality (Millipore Corp.)

Nanostructured TiO_2 films were prepared using the doctor blade technique,[20] depositing a layer (between 7 and 10 μm thick) of TiO_2 from a screen-printing paste (anatase titania nanoparticle paste, average size: 20 nm, Solaronix) on glass substrates.

The glass substrate was cleaned by sonication in a mixture of 2-propanol and acetone (50:50 v/v) and treated in O_2 plasma for 5 min at 50 W to remove the residual organic contamination. After deposition of the titania layer, the films were sintered at 500 °C (heating ramp 50 °C/min) for 1 h. The obtained TiO_2 film was further treated with UV-O_3 for 1 h or alternatively in O_2 plasma for 5 min at 50 W and then immersed in water. This step is useful for the removal of possible organic residuals and the enrichment of

Additionally, we studied the influence of thermal treatments on the prepared TiO_2 films. For this reason, samples of the series T500, TP500, and TPZ500 underwent a further heating treatment at 600 °C (50 °C/min) for 1 h. These samples were coded as T600, TP600, and TPZ600, respectively.

C. Samples characterization

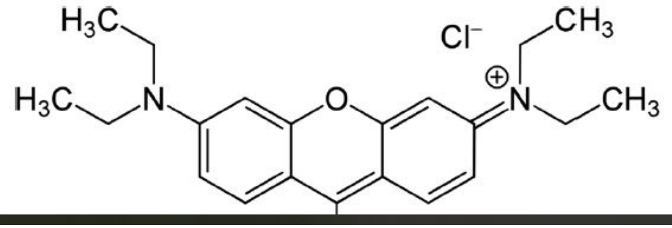
1. Structural and optical properties

XRD analysis was performed in a Smartlab Rigaku diffractometer in the Bragg–Brentano mode, equipped with a rotating anode of Cu Kα radiation operating at 45 kV and 200 mA. The average size of the crystalline grains was estimated from the XRD diffractogram using the Scherrer formula.[22]

The UV-Vis diffuse reflectance spectra (UV-Vis DRS) were carried out with a Jasco V-750 spectrometer equipped with an integrating sphere, using barium sulfate as reference. The optical bandgap of the samples was determined using the Kubelka–Munch function.[23]

2. Photocatalytic screening of TiO_2 films

A preliminary screening of different TiO_2 films under investigation was performed to determine the photocatalytic activity assuming first-order kinetics for the photocatalytic degradation reaction of RhB (Fig. 1) in solution.[24]



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Data to support the LabConnect project

Articles	Authors	Article Funding References	Article Study Details	Instruments	Materials	Theory / Simulation	Facilities
• Title • Journal name • Doi • Pub date • Instruments reference • Materials reference • Experiment techniques • Theoretical / simulation techniques • Funding references	• Author name • Orcid • Affiliation institution • Institution classification (Carnegie, HBCU) • Department • Address • Contact • CRediT reference • Tool expertise	• Funding reference • Grant number • Acknowledgement references • Facility reference • Facility funding references	• Research type (experimental, theoretical/simulation, or both) • Research problem statement • Finding summary	• Instrument name • Instrument PID* • Instrument details (settings / range) • Instrument supplier name • Instrument technique • Authors who oversaw use • Facilities • Facility PID* • Articles that reference	• Material name • Material PID* • Material source • Material usage details for reproducibility • Articles that reference	• Theoretical technique / model name • Software or algorithms used • Computational requirements and details • Articles that reference	• Facility name • Facility PID* • Facility location • Facility type (user facility, federally funded) • Facility/instrument funding references • Open status • Usage agreements • Usage fees • Instruments / capabilities • Research articles linked to work at the facility • Availably details • Staff contacts • Forthcoming tools

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*Note: Persistent identifiers (PIDs) will be developed to disambiguate facilities, materials, and instruments names. Where available we will utilize existing data sets for identifiers

The importance of PIDs for this work

Relevancy of PIDs to the project

- Can provide a structured data framework for disambiguating facility and instrument data
- Facilitates data verification in submission process - ideally like Dryad with facilities and RRIDs has done with reagents
- Creates opportunities for collaboration and coordination of data with facilities, funders, and other publishers

Thoughts on keys for success

- Clear use cases and benefits for stakeholders in research ecosystem
- Should be multidisciplinary – across STEM fields
- Critical for facilities to be a leading force in supporting metadata linked to PIDs
- Needs to be supported by funders, agencies, scholarly publishing ecosystem
- PID assignment needs to be seamless for authors

Response to Draft Recommendations

- The use cases - **traceability/citation, discovery, credit, reproducibility, provenance of research data** - are all critically important to publishers and the way we share scientific advances and support researchers
- The level of granularity needed for publishers is guided by what is relevant to communicate the research to others. In nano research – there are many bespoke instruments with unique calibrations and capabilities – so more granularity is likely needed
- Publishers have a role in utilizing PIDs and including them in our metadata
- Opportunity for capitalizing on author attention to data validation at submission – but publishers are weary of adding more barriers for authors. Need carrots and simple UX for verification.
- Publishers, researchers, funders, facilities will benefit from PIDs for facilities and instruments – but implementation path needs to be clear

Thank You`

msegers@aip.org

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