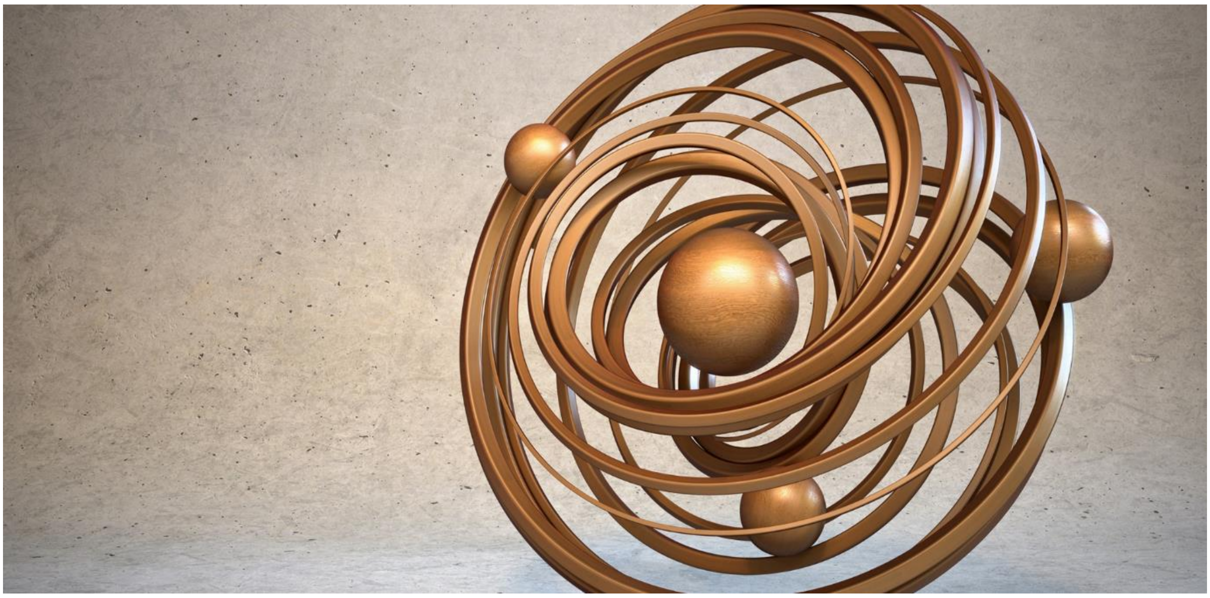

Molecular and Material Design Technology hub

Faculty of Science, University of Amsterdam

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1. Introduction

The global COVID-19 pandemic and the climate emergency underscore the urgency for accelerating cycles of scientific discoveries. Tools such as artificial intelligence, computational modelling and high performance computing and robotic automation are revolutionizing these scientific discovery cycles by breaking longstanding bottlenecks. Scientific progress has historically been driven by paradigm shifts in technology, from empirical studies to big-data-driven science. The current era emphasizes the synergy of heterogeneous capabilities rather than any single technology.

A typical discovery process can be decomposed into a series of events: (1) specification of a research question or a curiosity based surprise, (2) collection of data, (3) formation of a hypothesis and finally (4) experimentation and testing of this hypothesis. While this may seem conceptually simple, several significant challenges may hinder scientific progress. These include a.o. navigating vast design spaces, and ensuring reproducibility.

The inclusion of AI, modeling and experimental automation is key to accelerate and enrich all stages of scientific discovery (see figure 1). The vast discovery space can be expanded or reduced effectively by cycles of experimentation, data analyses and the use of generative AI models that offer new solutions to be tested experimentally.

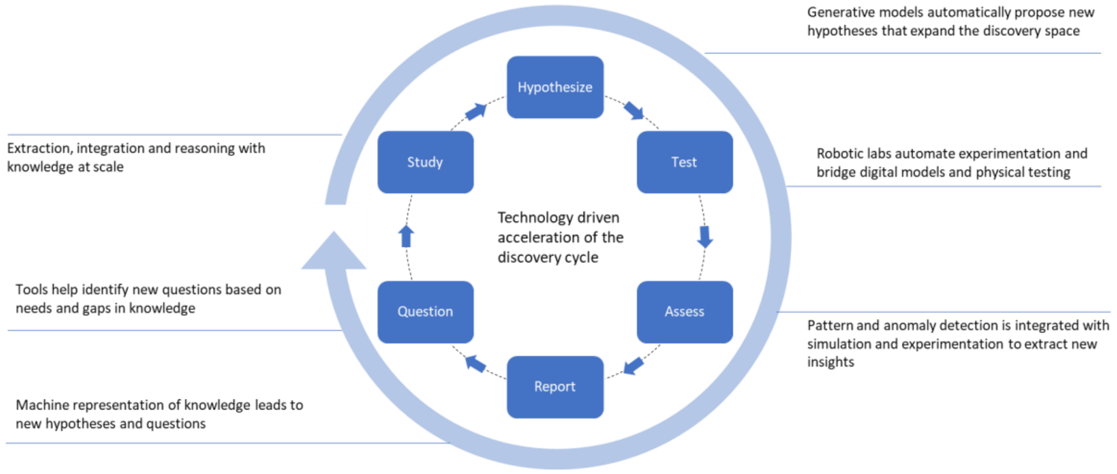
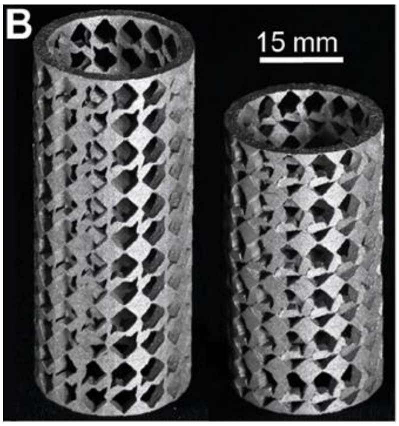


Fig. 1. Technology-driven acceleration of the discovery cycle (Pyzer-Knapp et. al. *Nature Computation Materials* 2022).

Many of today's scientific and societal challenges require new materials or molecules with tailor-made properties, whether it concerns applications in health care, the energy transition, circularity or mitigating climate change or advances in instrumentation for basic research. Novel materials and molecules with high-tech features need to be designed and produced effectively, economically, and with a minimal impact on our environment. At the Faculty of Science (FoS) UvA we are in the unique position to both develop and apply technology to speed up the scientific discovery cycle and to subsequently use such cycles in technological research to design new molecules and materials with potential strong impact in current societal challenges.

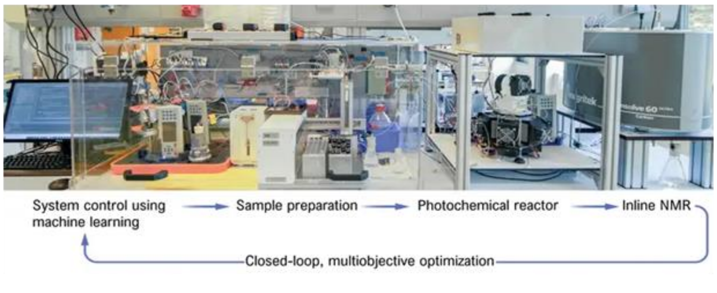
The FoS UvA therefore launches the Molecular and Material Design Technology hub (MMD) initiative to accelerate the discovery of materials and molecules critical to solving major societal challenges by implementing and developing new technologies across disciplines to expedite translation of the discovery process to the market. MMD understands technology broadly as: 'The application of scientific knowledge, principles, and methodologies to create, develop, and utilize tools, techniques, and systems that facilitate research, experimentation, analysis, and innovation across disciplines. Technology thus encompasses a wide range of hardware, software, processes, and methodologies aimed at solving the most complex problems, advancing knowledge.'



Example of a metamaterial combining properties (high strength and high dissipation) that are usually challenging to combine. The specimen has been 3d printed in stainless steel at the Faculty of Science. The innovation was made in the context of a NWO TTW project (Materialen NL) with industrial partners in the automotive and aerospace sectors, to investigate energy dissipation in mechanical metamaterials. This program resulted in a fundamental discovery of a new regime of the buckling instability that occurs for realistic materials such as steel. The program resulted in a patent and data reported in arXiv:2310.04748. Many open questions remain to optimize the performances of these metamaterials using AI techniques.

The ambition of MMD is to deploy and strengthen technology-driven acceleration in the discovery process within the FoS delivering technological solutions in both the Health and Green research themes addressing the Sustainable Development Goals and the objectives of the EU GreenDeal. We leverage our expertise in Pure and Smart themes to accelerate and create an impactful molecular and material design as the focus area for our Technology profile. As a result, both Tech4Science (instrumentation) and Science4Tech will be involved.

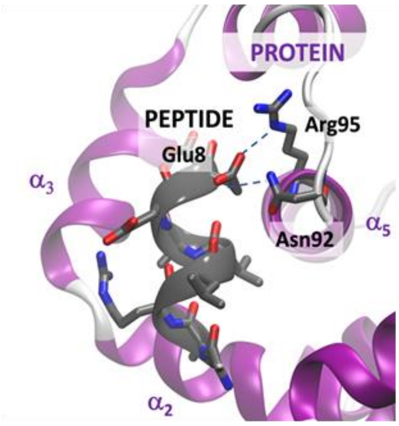
Developments in research and education are closely linked. For this reason MMD will be connected to future and ongoing educational initiatives in our BSc and MSc portfolio, including new initiatives such as the Science, Innovation and Technology BSc, the Origin InterSpecial minor (linked to the Amsterdam Center for Origins of Life, AMCOOL), and the course on emerging phenomena developed in the Foundations and Applications of Emergence (FAEME) research priority area.



Example of an autonomous chemical synthesis robot with an integrated AI-driven machine learning unit, developed by Chemists of the Faculty of Science (UvA). Dubbed 'RoboChem', the benchtop device can outperform a human chemist in terms of speed and accuracy while also displaying a high level of ingenuity. As the first of its kind, it could significantly accelerate chemical discovery of molecules for pharmaceutical and many other applications. RoboChem's first results were published on 25 January in the journal Science DOI: 10.1126/science.adj1817.

For the FoS it is imperative that we embrace our technological potential, which will require an investment at four levels:

- To build a thriving community that explores new opportunities and capabilities within the Faculty and its partners;
- To team up experimentalists, theoreticians, data scientists, AI experts, modelers, and technicians around research projects on molecular and material design;
- To permit a seamless access to state-of-the-art computational infrastructure with expert support;
- To enhance the experimental facilities for the generation and deployment of high-throughput data.



Example of a novel neuroprotective peptide for the treatment of Parkinson's disease. Parkinson's disease involves the loss of dopamine-producing neurons in the brain, leading to motor symptoms. Halting neurodegeneration would mean a major breakthrough in the treatment of this disease. In previous studies a key protein involved in neuronal survival was identified. Subsequently, a small peptide was generated which mimics the survival role of this protein. This approach combined rational design, artificial intelligence (AI) predictions, molecular dynamics simulations and experimental work. This project, a collaboration between SILS and HIMS, may provide the molecular basis for the design of novel anti Parkinsons's disease peptide-based therapeutics.

2. Mission & Vision

The mission of the MMD hub is to create a thriving community of scientists and partners (industry, government, society) that execute top-notch highly impactful technological research in molecular and material design. The hub will therefore function as an accelerator for research, by bringing together talent, tools and large data that enables us to close the cycle of fundamental knowledge, experimentation, data analyses and the design of new materials, molecules and associated processes.

The vision is that by establishing the MMD hub, we will combine our long-standing expertise in chemistry, physics and the life sciences with our strengths in AI and computational data, and quantum information sciences, which includes quantum sensing and quantum computing. Such unique combination of expertise in eight Faculty institutes represents a strong interdisciplinary research ecosystem that offers great potential for highly disruptive science and technology.

The expected impact will enable us to:

- Strengthen our unique position at the science–technology interface;
- Enlarge our external funding opportunities;
- Originate consortium leadership possibilities;
- Enhance the collaboration with public and private partners;
- Make the UvA/FoS a transformative environment for future talent and collaboration.

3. MMD Structure and Governance

The governance structure of the MMD Technology hub program is designed to ensure transparency, accountability, and foster a culture of collaboration, innovation, and excellence in research. The program will be overseen by a MMD Program Board (5-7 members) comprised of representatives from the FoS research institutes, and relevant stakeholders. This MMD Program Board will be responsible for setting strategic direction, approving research initiatives, and monitoring progress towards program goals.

Additionally, a daily Management Team will be established to provide day-to-day oversight and management of program activities. A Scientific Director (0.4 fte) and Program Manager (0.8-1.0 fte) will form the daily management. Regular meetings of the MMD Program Board and Management Team will be held to review progress, address challenges, and make necessary adjustments to the program strategy.

Based on their expertise, an external Advisory Board (3-5 members) provides advice, recommendations, and strategic guidance to the MMD Program Board overseeing the research program. The Advisory Board will provide insights into emerging trends, opportunities, and challenges in relevant scientific fields and societal issues, helping to shape the direction and priorities of the MMD Technology hub agenda.

An ad hoc assessment committee consisting of one MMD ambassador per institute will be formed to assess the applications of the MMD Impulse funding call (see below) and advice the faculty board.

4. MMD support schemes

The Molecular and Material Design hub consists of the following starting initiatives:

1. MMD Community & Partnerships – Coordination and support actions for strengthening connections, visibility, and creating and nurturing the community with events and get togethers organized at a lively physical meeting place where MMD fellows, project leaders link up to stakeholders in Amsterdam and beyond.

2. MMD Impulse – Open impulse funding calls (see below) to help establish already emerging collaborations, small grants from 50-150 k€ each, directed towards combinations of scholars. Focus on developing new ideas to a next phase, for instance by proof-of-concepts.

3. MMD Compute – Facilitate access to computational facilities (additional HPC to be added this year) and create a dedicated MMD compute support team of highly qualified technicians/scientific developers/e-science engineers for implementing computational models and machine learning or other workflows.

4. MMD Data – Investments in enhancing the experimental capabilities (both in hardware and technicians) to generate (or sometimes outsource?) (high-throughput/big) data needed to close the research cycle. Initially at a modest scale connected to the existing research space (at HIMS, IoP, SILS, IBED), but with the ambition to attract additional funding to build self-driving labs for a quantum leap in the experimental space covered.

4a. MMD Community & Partnerships

Building a vivid community is the primary ambition of the Molecular and Material Design Technology hub. To this end an open space will be created in collaboration with Sustainalab located in Matrix One where FoS researchers can meet and interact at one or more fixed moments in the week. The close proximity of Matrix One allows a direct connection to the highly specialized labs at the various FoS institutes (IoP, HIMS, SILS, IBED).

The core of the Molecular and Material Design Technology hub will be formed by Technology Fellows. These Technology Fellows are part time scientific or support staff or full time PhDs, PDs, lab technicians, scientific programmers, etc., as well as external collaborators that contribute to the development of a strong knowledge-based community.

To strengthen the partnership portfolio, the Molecular and Material Design Technology hub will, with help of a MMD business developer (recruitment is ongoing), seek strategic collaborations with major tech, chemical and material companies worldwide, and create public–private partnerships using e.g. the ICAI model as a best practice example. The MMD hub in Amsterdam will build strong relationships within the Amsterdam Ecosystem (e.g. with HvA, VU, Amsterdam UMC, ARCNL, AMOLF) in education, in co-creation with companies located in the Amsterdam region, and in national and international consortia.

4b. MMD-Impulse funding call

The MMD Impulse call aims to establish and further strengthen emerging collaborations that combine theoretical, experimental, analytical/instrumentation and computational/AI expertise in the field of molecular and material design. The proposed research should focus on molecular and material design creating impact in the FoS themes Health and/or Green. Applications should contribute to accelerating change through initiatives that are not yet happening elsewhere in FoS and/or are not easily funded via other channels. Ideally applications increase opportunities for external funding. A (first) round of funding is made available by allocating the '*stimuleringsgelden'* in 2024. Note that this has implications for who may apply, the size of the budget of the applications and how the budget can be spent. The eligibility criteria will be:

1. The MMD Impulse call aims to establish and further strengthen emerging collaborations that combine theoretical, experimental, analytical/instrumentation and computational expertise in the field of molecular and material design;
2. Applications are encouraged to focus on (one of) the MMD subthemes 'Health' and/or 'Green', with a strong scientific base ('Pure') and making use of modern analytical and computational methods ('Smart');
3. Full, associate and assistant professors may submit an application if they have a tenured/ tenure track position; Please note that the main applicant needs to have a tenured position.
4. Preferably, 2 FoS research institutes are involved in the application;
5. Applications amount to a minimum of 50.000 euro and 150.000 euro maximum;
6. Funding may be used for a range of activities contributing to the mission and vision of the MMD Technology hub, such as (setting up) research projects, stakeholder engagement, outreach activities, appointment of temporary staff, material costs, proof of concept activities (e.g. testing, experimenting, demonstrating and validating an idea), preparation of

a large grant application, organizing an international workshop/consortium/seminar series, or the development of external collaborations (consortia);
7. Applicants are requested to only apply for the money needed for the specified goals;
8. The maximum duration of the project is 3 years;
9. As a component of good research practice, collected and/or generated data in the project must be adhered to the FAIR principles, so that they can be re-used and referred to.

Note that a separate but related initiative in development is a collaboration on vascular immunology, using *Van Meenen* funds (currently with Swammerdam Institute for Life Sciences (SILS), Institute of Physics (IoP) and Informatics Institute (IvI) involvement) plus potential co-funding from the UvA and Amsterdam-UMC.

4c. MMD Compute

By investing in a dedicated MMD compute support team we aim to empower researchers by providing them with the necessary infrastructure, computational modelling tools, and expertise to efficiently collect, manage, analyze, and visualize data. By leveraging cutting-edge technologies and best practices in data engineering, this team aims to accelerate the research and enable breakthrough discoveries across various domains.

The MMD compute support team will collaborate closely with researchers across various disciplines to understand their data needs and requirements. The team will also closely collaborate with the IT department and UvA Data Science Center to leverage existing infrastructure, resources, and expertise in implementing data engineering solutions. The mechanisms by which they will work is through a voucher system connected to MMD impulse or other projects.

4d. MMD Data

In MMD Data we aim for investments that contribute to closing ‘data gaps’ in the envisioned scientific discovery cycles. The goal is to facilitate seamless and automated/robotized generation of experimental data using standardized data formats that can be fed automatically into downstream computational workflows. And vice-versa, the output from computational and data workflows can steer further experimentation, again in an automated fashion. This should thus lead to fully closed and automated high-throughput discovery cycles, but also to ‘data and workflow’ lakes that store all data, computational models, and workflows in dedicated repositories and facilitate their re-use.

Investments in MMD Data still need to be further specified, depending on an analyses of user needs, already existing infrastructure components, and the facilities of our partners at Amsterdam Science Park or elsewhere. For instance, it could entail setups for parallel screening of many experimental combinations, high throughput image acquisition and analysis, or upscaling the capacity of existing analytical methods. External funding will probably also be needed for larger initiatives (e.g. from NWO).

Initiatives funded in the MMD Impulse program are preferably geared to create standardized data to kickstart the MMD data lake. MMD Data will work closely together with MMD Compute and the UvA Data Science Center.

5. Appendix, draft budget allocation

The initiative will initially be supported using a number of resources. Below is a preliminary account of the budget allocation, in kind and in cash.

	Source	Amount
Governance		
Scientific Director, 0.4 fte	In kind / FoS	k€ 60 py
Program Manager	FoS	k€ 80 py
MMD Community		
Fellows	In kind / FoS	
MMD Business Developer	FoS / IXA	
Physical space	FoS Sustainalab funding	
MMD Impulse		
Seed grants	Stimuleringsgelden	k€ 1500 / 3 yrs
A-UMC joint project	Van Meenen + CvB + FdG	k€ 3000 / 4 yrs
MMD Compute		
HPC	Van Meenen	k€ 1500
Support unit	FoS	p.m.
MMD Data		
Lab automation		p.m.
Datalake & Workflows		p.m.
Total		