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The Changing Landscape of Materials Discovery

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Abstract: In this perspective, we will discuss the impact of some of the most recent advancements in materials discovery, particularly focusing on the role of robotics, artificial intelligence, and self-driving laboratories, as well as their implications for the Swiss research landscape. While it seems timely to aim for broad, revolutionary breakthroughs in this field, we argue that more incremental steps – such as, for example, fully automatic grinding of solid powders or fully automated Rietveld refinements – may have a more significant impact on materials discovery, at least in the short run. In the center of these considerations is how small, interdisciplinary groups can drive significant progress by contributing targeted innovations, such as *e.g.* robotic sample preparation or computational predictions. Additionally, given the large investments that are necessary for future infrastructures in materials discovery, we discuss the potential case for the establishment – in the long run – of a national infrastructure, a Swiss Materials Discovery Lab, to support automated material synthesis and advanced characterization, ultimately accelerating innovation in both academic and industrial settings.

Keywords: Materials discovery · Self-driving laboratories · Solid-state chemistry

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1. Introduction

Material discovery has always been at the forefront of technological progress, driving the evolution of human civilization. The ability to identify, create, and utilize new inorganic materials has led to groundbreaking innovations across all industries, exemplified by rechargeable lithium-ion batteries powering portable electronics and electric vehicles,[1–3] stainless steel that transformed several industries like construction,[4] or silicon chips – enabled by nearly defect-free single crystalline silicon – that sparked the digital revolution.[5,6] Material discovery resulting from fundamental research in inorganic chemistry has always been tedious work.[7,8] This experimental research associated with trial and error, and extensive investments in strenuous and time-consuming laboratory work, has often been found to be slow and unpredictable.[9] With the advent of advanced technologies like artificial intelligence (AI), robotics, and self-driving laboratories, the landscape of material discovery is widely believed to be rapidly evolving, promising faster, more efficient breakthroughs.

The development of these technologies certainly aims to revolutionize many areas of chemistry research, they may, however, likely have one of the largest impacts on materials discovery. Recent advancements in AI and robotics have particularly highlighted their transformative potential in materials discovery, allowing for more automated, data-driven approaches to identifying and synthesizing new compounds.

AI is believed to revolutionize materials discovery by accelerating predictions, optimizing synthesis processes, and enhancing data analysis. For example, generative machine-learning models may learn from known material data to predict new material properties, and are also believed to enable the design of novel materials that were so far beyond the scope of experimentation. Moreover, AI may facilitate the analysis of data generated by characterization techniques. Robotic labs may automate many tedious and repetitive tasks such as sample weighing, mixing, and loading for synthesis, significantly speeding up processes that would otherwise be limited by manual labor. They are expected to eliminate variability caused by human error and allow for a consistent and reproducible execution of experiments, particularly useful in high-throughput workflows. Robotic labs equipped with AI may autonomously conduct and refine synthesis and optimize conditions and analysis ultimately resulting in so-called self-driving laboratories, see, *e.g.* refs. [10–15].

As we will discuss in detail below, two manuscripts, both published in Nature, have sparked, in particular, significant interest in AI and robotics-driven material discovery most recently.[16,17] The reported results may have been found to fall short of the acclaimed revolutions, but these recent developments have nonetheless ignited critical discussion within the scientific community, raising important questions about the true impact of these forthcoming developments.[18,19] In these discussions, the hurdles that must still be overcome before the anticipated revolutions can be realized, as well as the needs to be met with regard to essential infrastructures and the evolving nature of future collaborations required to support this progress is being outlined.[18,19]

Here, we will argue that while the allure of large, groundbreaking leaps in material discovery is undeniable, it may be more practical and potentially even more impactful to address some mundane challenges in material discovery first. For instance, robot-assisted synthesis preparation, such as the automated grinding and mixing of elements, the full automation of scattering experiments, and improved analysis tools for off-stoichiometries, would each significantly accelerate material discovery. By focusing on these foundational improvements, we can make substantial strides

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in the field. Moreover, accurate predictions, material synthesis and analysis remain major bottlenecks in the discovery process. AI-driven predictions may offer educated guesses on where to find new and interesting materials, nonetheless, the need for skilled chemists to create any material or at least supervise its creation remains critical for the foreseeable future. To address the pressing material challenges of our time, it is essential to advance both the technological tools available and the human expertise that drives innovation in materials science. In the long run, a Swiss Materials Discovery Lab as a national infrastructure might be beneficial for both academia, as well as industry, and it should be discussed in the context of national infrastructure planning. Such an infrastructure might work on a user/proposal basis in order to benefit many research groups.

2. Conventional Materials Discovery

Materials discovery is a multifaceted process, which we will focus on in the following sections, through the lens of our expertise in quantum materials discovery. The exploration primarily focuses on these materials and there are certainly differences when considering other material classes like battery materials or catalysts, but all these material exploration branches share many commonalities. It should be noted that, of course, there is a not too subtle distinction between the term materials and extended inorganic solids, even though we will use these terms interchangeably with a focus on the latter within this perspective.

One of the grand challenges in quantum materials lies in their particular sensitivity to subtle variations in lattice parameters, interaction distances, bond lengths, symmetries, atomic composition, and site occupancies, which are known to profoundly influence the properties of quantum materials.[20,21] Henceforth, high-quality samples using advanced synthesis and crystal growth methods are critical for advancements in this field and property predictions are still extremely challenging due to the emergent nature of the properties in these materials. For instance, as discussed in a recent perspective, discovering something as complex as a topological superconductor demands the precise alignment of various critical factors, all of which must converge to give rise to the desired emergent properties.[22]

In Fig. 1, we show a graphical representation of the common quantum materials discovery process. This is an adapted version from discussions that can also be found in refs. [7,8,23–27]. The basic steps are (i) *the targeting of a desired material property*. This can be, for example, a quantum spin liquid, a new superconductor, or a topological material. The next step is (ii) *the guidance step*, where certain materials that might display a desired property are being identified by an analysis of structural and electronic features. This step involves an in-depth analysis regarding the stability and chemistry of the targeted system.

This is done by chemical heuristics, supported by the assessment and conceptualization of known structural motifs and their chemical bonding, magnetic interactions, as well as electronic band structures. This step can be accompanied by stability, electronic and magnetic computational predictions. These analyses guide us towards a subset of materials that might be hosting the desired property.

These two steps are then followed by a feedback loop of steps that are (iii) *the (attempted) synthesis of new materials*, (iv) *the structural identification of the reaction products*, (v) *the characterization of the properties of the synthesized materials*, and (vi) *the development of models to describe the observed experimental outcomes*. The results of this feedback loop reiterate the previous steps, refined material predictions are made and they enter the cycle again. These processes are repeated until new material structures, new materials, or new properties are discovered, which then may result in the basis for *unprecedented material physics to be discovered*, step (vii). If applicable, these properties may then be refined so that eventually a *new device or application might potentially be realized*, step (viii).

These processes have not changed much over the years, and one of the major limiting factors in any material discovery remains today the lack of being able to rationally design inorganic solids. The review article '*A Concept for Synthesis Planning in Solid-State Chemistry*' by Martin Jansen from 2002 is as timely now as it was then.[7] Jansen discusses the fundamental obstacles in rationally designing solid-state reactions, such as the difficulty in controlling reaction pathways due to poor atomic-level mixing and high thermal activation requirements. He highlights that solid-state synthesis remains largely explorative, requiring innovative approaches for better control and predictability in creating new materials. Despite advances, issues like the limited predictive power of theoretical models and the challenge of selectively guiding solid-state reactions are still barriers to more systematic and rational material design. In fact, great advances in material discoveries often go along with advances in synthesis methodologies.[9] Nowadays, we see a surge in promising materials by the availability of soft-chemical methods that have enabled materials such as for example the van der Waals room-temperature ferromagnet $CrTe_2$,[28,29] or the van der Waals superconductor 2M-WS_2 with the highest critical temperature among the transition metal dichalcogenids to date.[30,31]

In his review article, Jansen argues that even with a high-throughput approach capable of producing 10,000 samples per day, discovering a complex material like $YBa_2Cu_3O_7$ (commonly referred to as YBCO) would still take an estimated 27,000 years. While the synthesis and analysis of 10,000 samples a day was in 2002, of course, still impossible, these numbers become more realistic in a robotic materials discovery lab. These considerations underscore that while automation and robotics can accelerate certain tasks, progress in solid-state chemistry and (quantum) materials discovery depends on overcoming also other challenges. Thus, the future of materials discovery will rely not only on automation, but also on integrating deeper chemical understanding and refined models.

3. Most Recent Advances

In AI and robotics driven material discovery, two recent publications in Nature have drawn considerable attention, proclaiming major breakthroughs towards the next generation of materials discovery.

Firstly, in November 2023, Merchant *et al.* from the Google GNoMe project described the use of AI and machine learning techniques to discover new inorganic materials.[16] These include traditional compounds like oxides and halides, as well as other main group compounds and intermetallics. They reported that they have identified, an astonishing amount of, 2.2 million structures below the current convex hull, many of which have eluded previous human chemical intuition. Nearly 400,000 of these structures were classified as stable and have been included in a Stable Structure database, while detailed information on over 2,000 of these new compounds has been added to the GNoME Explorer archive within the Materials Project.

Secondly, to speed up progress in materials discovery, a team at UC Berkeley has created an automated laboratory, which they call A-lab.[17] In their laboratory, they have integrated robotics and AI for this challenge, robots handle autonomously all the tasks of materials discovery, including things like mixing and heating ingredients, and measuring powder X-ray diffraction (PXRD) of the resulting products. An algorithm then interprets the PXRD patterns to determine whether the synthesis was a success or not. Then their workflow is adjusted to address the diagnostic feedback accordingly. This group announced in their much-noticed *Nature* paper that within a span of 17 days, the lab successfully synthesized 41 new materials out of 58 predicted targets.

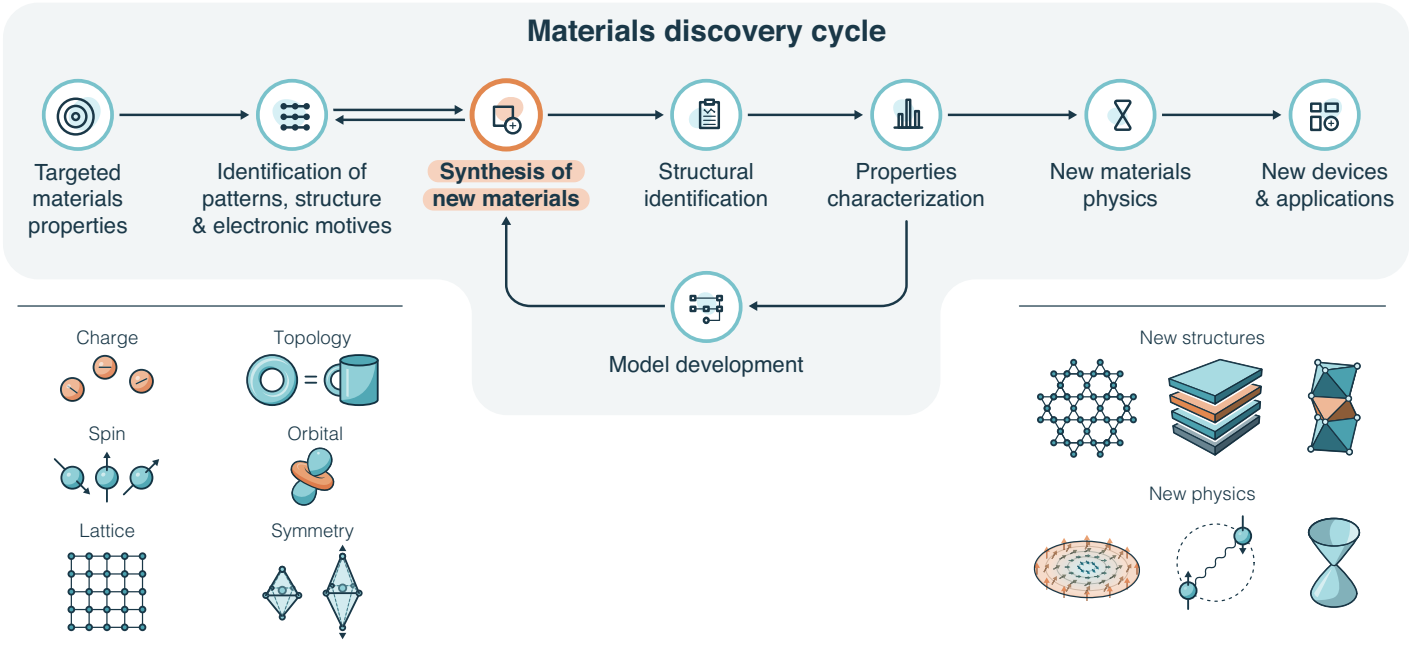

Fig. 1. The materials discovery cycle shows schematically how new materials are discovered and characterized, and how potentially new materials physics and eventually new devices result from them. On the bottom left the degrees of freedom are schematically shown and on the bottom right is a schematic representation of the new crystal structures and new physical properties that result from their combination.

Both, the results from GNoME, as well as the ones from A-lab have been met with scrutiny from the community.[18,19] In the following, we will briefly summarize the issues that have been pointed out regarding these publications:

(i) The GNoME results have been met with substantial criticism, particularly regarding these key issues:[18] Firstly, many entries in the GNoME Explorer database are lacking novelty, with compounds being mere variations of already known phases. Secondly, the database was found to contain vast amounts of improbable structural features, such as unrealistic oxidation states and excess anions, which raise doubts about the accuracy of the predictions. Given the vast amount of multi-elemental phases in the list, it is difficult to clearly see through the structures. But to get a general idea, we invite the interested reader to download some of the binary structures of the proposed materials, *e.g.* of GeI_{26} and $MoSe_{23}$.[32] Both of these compounds clearly violate basic rules of chemical heuristics that any chemistry undergraduate student could easily spot. Moreover, the frequent prediction of ordered structures where disorder is expected, particularly in compounds involving lanthanides, casts doubt on the reliability of GNoME's output. One of the examples Chethaam and Seshadri discuss in this regard,[18] is an η-carbide-type compound from the GNoMe manuscript, namely Zr_4Ir_2N, a known crystal structure registered in the ICSD under no. 640826. GNoMe proposed the new compound $Hf_4Ir_8N_4NbZr_{11}$ that has in reality the same structure, but all the transition metals are fully ordered on different sites. The novelty of this structure and composition is highly doubtful to any solid-state chemist.

We have worked on η-carbide-type compounds recently, and we have discovered them to be superconductors with remarkably high upper critical fields.[33–35] We found that the transition metal separation on the crystallographic sites is highly unlikely in these materials. In fact, even the stoichiometry of η-carbide-type compounds can be variable. The 'parent compound' of η-carbides is the Ti_2Ni structure, which crystallizes in the cubic space group $Fd\bar{3}m$ and contains 96 metallic atoms occupying three crystallographic sites on Wyckoff positions 16*d*, 32*e*, and 48*f*. The Ti atoms occupy the 16*d* and 48*f* sites, which form a network of distorted [Ti_6] octahedra. The Ni atoms are at the 32*e* position, forming a network of [Ni_4] tetrahedra. Ti_2Ni shares a close relationship with the η-carbide structures. The η-carbide structure can be understood as a filled version of the Ti_2Ni structure, where light nonmetallic atoms, occupy the 16*c* Wyckoff position (inside the octahedra). However, the η-carbide structure not only forms for the stoichiometry A_4B_2X, but also for the stoichiometry A_3B_3X (with *A* and *B* being transition metals, and *X* being a light element either O, N, or C). In these A_3B_3X *phases*, the *B* atoms occupying the 48*f* Wyckoff site, highlighting the very unlikely scenario that a fully ordered $Hf_4Ir_8N_4NbZr_{11}$ could be even remotely realistic. In a sense, the existence of a $Hf_4Ir_8N_4NbZr_{11}$-type phase as proposed, would be the antithesis to the existing and proven concept – that has also been found valid for quantum materials – of high-entropy alloys, where the high configurational mixing entropy allows for the stabilization of highly disordered, but simple structures, *i.e.* the atoms arrange on *pseudo* BCC, FCC or HCP lattices.[36–38]

While the proposed phase $Hf_4Ir_8N_4NbZr_{11}$ is at least close to a structure that might actually exist, there are vast amounts of structures that are far from any chemical heuristics. Chethaam and Seshadri come to the following conclusion in their analysis of the GNoME results:[18] "*We examine the claims of this work here, unfortunately finding scant evidence for compounds that fulfil the trifecta of novelty, credibility, and utility. While the methods adopted in this work appear to hold promise, there is clearly a great need to incorporate domain expertise in materials synthesis and crystallography*."

(ii) The A-lab project, which claimed to have discovered 43 new materials using automated robotics and AI, has encountered significant criticism from the scientific community. For any inorganic chemist who is discovering new materials, major concerns can easily be raised about the accuracy of the interpretation of these results. For one, it is immediately clear that many of the claimed new materials appear to be misclassified versions of existing known compounds. Secondly, the automated Rietveld analysis employed by A-lab – a result that would be a major scientific achievement by itself, if true – is clearly unreliable, leading to incorrect characterizations. The automated Rietveld refinements performed by A-lab were found to be leading to inaccurate fits of the PXRD data. In several cases, key diffraction peaks were either entirely missed or misinterpreted, which casts doubt on the accuracy of the structural conclusions drawn. Another concern

are impurity phases in the samples, as A-lab's results showed incomplete reactions and unreacted starting materials in numerous cases. Thirdly, the lack of consideration for disorder in crystal structures has further undermined the credibility of the reported findings. One major issue raised is that many of the compounds claimed as 'new' are more likely disordered versions of already known materials, rather than truly novel discoveries. This misclassification stems from inadequate consideration of compositional disorder, which is often overlooked in both prediction and refinement processes. Fourthly, a further significant issue with the A-lab results is related to the misinterpretation of cation ordering. In many cases, it was claimed that a new material with ordered cations was synthesized, such as *e.g.* $MgTi_2NiO_6$, but a detailed analysis revealed that the experimental diffraction data matched disordered phases already known in the literature. For instance, Leeman *et al.* found that in the case of $MgTi_2NiO_6$, the predicted ordered structure was not supported by the PXRD pattern, which was better explained by the known disordered ilmenite-type phase.[19] This misinterpretation extends to other materials, where predicted ordered structures often turned out to be disordered versions of existing compounds. Leeman *et al.* come to the following conclusion in their detailed analysis of this work:[19] "*We discuss all 43 synthetic products and point out four common shortfalls in the analysis. These errors unfortunately lead to the conclusion that no new materials have been discovered in that work.*"

While the claims made by these projects may so far have fallen short of their ambitious promises, they have undoubtedly sparked important discussions in the field of materials discovery. These initiatives have drawn attention to the challenges and limitations of applying AI and robotics in the complex realm of solid-state chemistry, highlighting the need for greater collaboration between computational predictions, automated processes, and human expertise.

4. Realistic Short-Term Goals

It is evident that both of these general trends – robotic laboratories and advanced computational predictions – will play a pivotal role in the future of materials discovery and solid-state chemistry. There are currently three significant obstacles slowing down high-throughput materials discovery. The first challenge lies in the prediction of new materials, where the balance between speed and accuracy in calculations has yet to be fully resolved, *i.e.* steps (i) and (ii) in the materials discovery process discussed above. The second hurdle involves sample analysis, *i.e.* steps (iv) and (v) in the materials discovery process. The third major challenge is ensuring efficient and targeted sample preparation. However, it is important to emphasize that simply increasing the number of samples does not necessarily accelerate the materials discovery process. Instead, success depends on the strategic selection of experiments and the analysis of the performed synthesis, where quality and relevance take precedence over sheer quantity. Effective sample preparation should focus on optimizing conditions and ensuring reproducibility, allowing chemists to explore meaningful variations in material properties, rather than overwhelming the process with excessive, unguided sample production.

While it is impressive to autonomously predict and produce numerous samples, if the bottleneck remains in human-operated analysis, then an AI-driven robotic lab may not be any faster than the slow traditional methods. Although there have been significant advances toward unsupervised analysis, we believe that truly autonomous material analysis is still a goal for future research, and an improved human-machine interface could significantly accelerate the process.

It would be desirable to have advanced computational tools and robotic support in the laboratory in order to achieve faster, more targeted materials discovery, however, for now, it might be more beneficial to first overcome more mundane challenges that arise to experimental chemists in this field. In the following, we present a wish list (in no particular order) of improvements. This list is certainly not exhaustive, and it might look different for other areas of materials discovery.

(i) *Robotic Weighing of Reactants*

Automating and increasing the precision of reactant quantities is a critical advancement for streamlining experimental workflows in materials discovery. By integrating robotic systems to accurately weigh and dispense reactants, we could reduce error, improve reproducibility, and – most importantly – significantly reduce preparation time. This is especially important in the context of higher throughput synthesis.

(ii) *Automatic Grinding of Solid Powders*

Robotic systems designed for automatic grinding might ensure consistent particle size and homogeneity in solid powders, but also significantly reduce preparation time, as grinding is a major mundane hurdle that any solid-state chemist has to deal with. In traditional manual grinding processes, variations in particle size and mixing uniformity can lead to inconsistencies in experimental results, particularly in solid-state chemistry where many reactions are diffusion limited and occur at the grain boundaries.

(iii) *Automatic Pellet Pressing*

Robotic equipment for pressing powders into pellets plays a crucial role in ensuring uniformity and precision in sample preparation, while speeding up the process. This is particularly important in solid-state chemistry, as again many reactions are diffusion limited.

(iv) *Automatic Sealing of Quartz Tubes*

Automated tools for sealing the reactants in quartz tubes under inert atmosphere are essential for any non-oxide material synthesis. Automated sealing minimizes error, increases safety by reducing direct handling of hazardous materials, and speeds up the preparation process.

(v) *Modular Synthesis Equipment*

Modular synthesis systems enable several consecutive synthesis steps to be performed in a straightforward and integrated fashion, allowing us to switch between different synthesis methods – such as solid-state reactions, hydrothermal processes, or vapor-phase techniques – without requiring extensive reconfiguration. Such flexibility would improve the efficiency of multi-step synthesis workflows.

(vi) *Robotic Scattering Measurements*

Full automation of sample preparation and performance of PXRD and SXRD (single-crystal X-ray diffraction) experiments would increase the efficiency of crystallographic analysis. Such robotic systems should be able to autonomously prepare the samples for measurements, load them into the diffractometer, and execute the entire measurement process, including data collection and processing. By automating these XRD experiments, we could dramatically accelerate the characterization of new materials.

(vii) *Fully Automatic XRD Analysis*

Automated systems should be able to quickly and accurately perform Rietveld refinements for PXRD data, as well as find solutions and perform refinements of SXRD data. By automating these processes, researchers can achieve faster, more consistent results, while minimizing errors. Such systems should be able to automatically handle complex refinements, including phase identification, lattice parameter determination, and atomic position refinement also for multiphase systems.

(viii) *Improved Soft-chemical Synthesis Set-ups*

To bring soft-chemical synthesis for materials forward, systems will need to go beyond the traditional Schlenk line, integrating automation, and precise synthesis condition control. Such systems could for example feature automated reagent handling and dosing to ensure exact quantities, while reaction vessels equipped with temperature and pressure control might allow for diverse synthesis conditions. Soft-chemistry methods for material synthesis will be essential to integrate in robotic labs as these methods allow for overcoming many current limitations in solid-state chemistry.

(ix) *Improved in situ Characterization Tools During Synthesis*

Integrating easy to use precision *in situ* characterization tools into the synthesis process may allow for real time monitoring of the reactions as they evolve. This may provide insights into key aspects such as phase formation, crystallization, or structural changes, enabling us to dynamically adjust synthesis conditions for optimal outcomes. By observing these changes as they occur, we could better understand reaction mechanisms, improve reproducibility, and fine-tune experimental parameters.

(x) *High-throughput Compositional Analysis*

Techniques for rapid and precise compositional analysis are essential in materials discovery. Incorporating high-throughput methods such as Energy Dispersive X-ray Spectroscopy (EDX), Inductively Coupled Plasma Mass Spectrometry (ICPMS), X-ray Photoelectron Spectroscopy (XPS), and Rutherford Backscattering Spectrometry (RBS) would greatly enhance the accuracy and reliability of material characterization.

(xi) *Simultaneous Characterization Tools*

Integrating simultaneous characterization techniques, such as *e.g.* EDX and diffraction experiments in a single easy to use device, would offer a powerful approach to gain comprehensive insights into synthesis products. Combining such methods would allow us to obtain detailed information about both the structural and compositional aspects of a single grain of a material in a single experiment.

(xii) *Automated Single-Crystal Growth*

Developing automated systems for the growth of high-quality single crystals, using different methodologies, including flux, vapor transport, Czochralski, or Bridgman growth techniques would be a significant advancement in materials discovery. Single-crystals provide clearer, more interpretable data for structural analysis and enable precise measurement of the anisotropic physical properties, substantially improving our understanding of matter. Automation in this area could streamline the process of crystal growth, making high-quality crystals more accessible for a wider range of materials and eventually also for applications.

(xiii) *Precise Prediction of Inorganic Structures*

The development of accurate computational models for predicting stable inorganic structures remains one of the key challenges in computational materials discovery. This is even true for binary, ternary, and quaternary systems, despite major investments in the past. These computational models should aim to predict the thermodynamically stable configurations of elements. Also, especially helpful, would be the ability to predict dynamics and stabilities for these systems starting from atomic and molecular building blocks, in order to point towards accessible synthesis pathways.

(xiv) *Prediction of Defect Chemistry*

Developing computational tools to accurately predict defect behavior and off-stoichiometries within materials is crucial for understanding and optimizing material properties. Defects, such as vacancies, interstitials, and substitutional impurities, often play a pivotal role in determining a material's electrical, optical, magnetic, and catalytic properties. For instance, in semiconductors, the presence of defects can affect charge carrier mobility, while in catalysts, they can influence reaction sites. Predictive models that simulate defect chemistry should account for complex interactions at the atomic level, including the energetic favorability of defect formation, their diffusion, and how they alter the local electronic structure.

(xv) *Property Calculations for Off-Stoichiometric Materials*

Developing reliable methods for accurately modeling non-stoichiometric systems is crucial for understanding real-world material behavior, where perfect stoichiometry is often unattainable. These off-stoichiometric materials often have deviating properties from the calculated ideal chemical ratio compounds, which ultimately can, for example, significantly impact their performance in electronic devices.

(xvi) *Collaborative Data Management*

Collaborative platforms for data storage and analysis may become essential for modern materials discovery. As the amount of data generated in high-throughput experiments and automated synthesis will grow, efficient data management systems are needed to store, organize, and analyze these large datasets. These platforms should allow us to easily share and access experimental data, promoting collaboration across different labs.

It should be noted that all of these approaches, to be truly helpful need to be able to be performed under inert conditions, something that does not seem impossible but that – to the best of our knowledge – has only been discussed scarcely so far. These goals might seem more mundane than the proposed goals of achieving self-driving laboratories right away. However, each one of these steps still represents a major milestone and would – if achieved – result in a major leap forward for the field of materials discovery. It is important to remember – even though it might seem obvious to most – that new materials can only be truly considered 'discovered' once they have been successfully synthesized and thoroughly analyzed in a laboratory. Theoretical predictions and computational models are valuable tools for aiding discovery on different levels, but without physical validation, these materials remain speculative. Therefore, adequate support should be allocated to the experimental aspect of materials chemistry.

It should also be noted that for many of the points on this wish list, there have been achievements recently that make us hopeful that some of these helpful tools might be available in a not too distant future. There exist proposed technical solutions to many of these points, though they may be limited in scope, require adaptation, or are often specialized for other applications. For example, recent progress in machine learning applications for XRD analysis, such as the work by Danna Freedman's group, points towards a promising future in fully automated PXRD refinement.[39] Or, dispensing of solids is offered by several equipment suppliers, each with their own unique technologies and strengths. However, these existing systems may need further refinement to meet the specific demands of materials discovery under strictly controlled conditions. Solutions to automated grinding, sieving, and pelletizing are to some extent commercially available and might be adapted for materials discovery in the future. Moreover, some equipment providers already offer modular synthesis platforms that allow for multiple synthesis methods – including *e.g.* precipitation and hydrothermal synthesis on a single machine. Many of these developments hold great promises. Importantly, feasibility of the many possible technologies, their evaluation, implementa-

tion, and common integration cannot be practicably undertaken by every individual research group. This is where a common materials discovery infrastructure, as discussed later in this article, might also become essential.

5. Materials Discovery in Switzerland

What do these developments mean for materials chemistry and materials discovery in Switzerland? These are promising developments for the Swiss community. Materials discovery, which has a tremendous impact on society, is entering a new era. However, these changes appear to be happening more slowly than initially promised. It seems that small, collaborative groups sharing their expertise will have the most profound impact. Strong individual research groups contributing specific steps – such as robotic intermediary preparation or computational material predictions – will be key within these collaborations.

In the long run, it seems challenging that fully equipped robotic laboratories for materials discovery will be established at every institution in Switzerland, as their realization would likely require massive investments. The high costs involved in acquiring advanced automation systems, maintaining the equipment, and integrating AI-driven tools are considerable. Additionally, the operation of such laboratories requires substantial investment in specialized personnel, both for engineering the infrastructure and managing its ongoing operations. However, given the necessity for academia and industry to have access to such systems, a common Swiss Materials Discovery Lab should be considered as an option. Such a facility could serve as a shared, national resource, offering access to state-of-the-art robotics, high-throughput synthesis platforms, and advanced characterization tools to researchers from both academic and industrial sectors.

By pooling resources into a single, well-funded infrastructure, we could avoid the inefficiency of duplicating costly equipment across multiple institutions. This approach could not only ensure broader access to cutting-edge research capabilities but could also foster collaboration across sectors. Such a common facility could be driving forward research and technological advancements.

Such a Swiss Materials Discovery Lab could be considered among the next generation of large-scale facilities for the community. It could be a proposal-based facility similar to other shared large-scale facilities. This infrastructure could allow, for example, for ordering prepared reactions from a robotic lab combined or advanced computational analysis tools. A Swiss Materials Discovery Lab could be envisioned as an implementation and progression of the PARADIM (Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials) platform funded by the National Science Foundation in the United States, where already today resources are shared in the US community in order to implement a closed loop Materials-by-Design process to discover novel materials. Other inspiration might be drawn from the SwissCat+ initiative from ETH Zürich and EPFL. This national infrastructure project – as part of the Swiss Chemistry Roadmap – aims at combining highthroughput and automated experimentation platforms as a centralized, open-access facility, for efficient screening of catalytic reactions. As an open-access facility, SwissCAT+ aims at supporting researchers across Swiss institutions, offering them access to high-throughput tools and expertise.[40,41] Similarly, other institutions in Switzerland have developed initiatives focused on specific areas of robotic laboratories and AI integration in discovery. For example, EMPA has launched a high-throughput platform for catalysis and battery research,[42,43] within the NCCR MARVEL the AiiDA platform was developed for scalable computational infrastructure for automated workflows,[44] and the University of Zurich has initiated the development of a high-throughput lab for the synthesis of a broad catalyst library. In addition to these efforts, collaborative data management initiatives such as the CHORD program, driven by swissuniversities and the ETH domain, are aiming to support efforts towards a unified data infrastructure in Switzerland.

Drawing from these developments, and given the critical role materials discovery and optimization play in society, providing such infrastructure for the purpose of materials discovery – *e.g.* as a Swiss Materials Discovery Lab – to the Swiss community might be essential.

6. Conclusion

In this perspective, we have explored the evolving landscape of materials discovery, particularly focusing on the integration of advanced technologies like robotics, AI, and automation. While these innovations hold great promise, especially within the realm of quantum materials discovery, their full potential has yet to be realized due to several critical challenges. Notably, targeted advancements in experimental processes – such as: robotic sample preparation; automated scattering analysis; and the precise control of solid-state synthesis – must take priority to accelerate discovery and ensure reliable outcomes.

Furthermore, the automation of routine tasks like sample weighing, grinding, and data analysis might significantly improve efficiency in laboratories, but the mere increase in the number of samples is not a substitute for smart, strategic experimentation. It is the strategic design of experiments that will drive impactful discoveries.

Lastly, we propose that – in the long run – a national infrastructure, such as a Swiss Materials Discovery Lab, could provide essential support for both academic and industrial researchers. By offering shared access to advanced specialized tools and methodologies, this infrastructure might enable the scientific community to contribute more effectively to innovations in materials science.

In summary, while the future of materials discovery lies in automation and AI, the immediate focus should be on overcoming the foundational challenges in synthesis and analysis, which will ultimately pave the way for the rapid development of new materials and their applications. Certainly, the outlook for materials discovery is promising, with significant advancements on the horizon, driven by innovations in the field.

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