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Perspective

Designing durable, sustainable, high-performance materials for clean energy infrastructure

Jason Hattrick-Simpers,⁴ Kangming Li,⁴ Michael Greenwood,² Robert Black,³ Julia Witt,¹ Mark Kozdras,² Xin Pang,^{2,*} and Ozlem Ozcan^{1,*}

SUMMARY

Civilization and modern societies would not be possible without manmade materials. Considering their production volumes, their supporting role in nearly all industrial processes, and the impact of their sourcing and production on the environment, metals and alloys are and will be of prominent importance for the clean energy transition. The focus of materials discovery must move to more specialized, application-tailored green alloys that outperform the legacy materials not only in performance but also in sustainability and resource efficiency. This white paper summarizes a joint Canadian-German initiative aimed at developing a materials acceleration platform (MAP) focusing on the discovery of new alloy families that will address this challenge. We call our initiative the “Build to Last Materials Acceleration Platform” (B2L-MAP) and present in this perspective our concept of a three-tiered self-driving laboratory that is composed of a simulation-aided pre-selection module (B2L-select), an artificial intelligence (AI)-driven experimental lead generator (B2L-explore), and an upscaling module for durability assessment (B2L-assess). The resulting tool will be used to identify and subsequently demonstrate novel corrosion-resistant alloys at scale for three key applications of critical importance to an offshore, wind-driven hydrogen plant (reusable electrical contacts, offshore infrastructure, and oxygen evolution reaction catalysts).

INTRODUCTION

According to the IMPACT study by NACE International (now called the Association for Materials Protection and Performance), the global cost of corrosion is estimated to be \$2.5 trillion USD, equivalent to 3.4% of the global gross domestic product (GDP) at the time of the study in 2013.¹ It is not only an enormous economic burden but is, more importantly, a safety risk both for people and the environment. For a sustainable future, we need to design materials that retain their integrity and functionality over much longer timescales than we can imagine today. Moreover, beyond the scope of the IMPACT report, which focused solely on structural materials, the hidden cost of material degradation in the renewables sector, be it electrolyzers, fuel cells, hydrogen infrastructure, or batteries, will dramatically impact these estimates and lead to resource availability and recycling problems in the near future. Thus, corrosion-resistant, durable materials will be one of the hidden enablers of the clean energy transition.

We believe that our material world today is built upon a relatively small set of material systems, most of which are legacy materials not tailored for today's applications.

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This is a sector- and material-class-independent reality and has some legitimate reasons for being so. Financial reasons, both in terms of material and development costs, is one main driver of this phenomenon. The most prominent example is the decades-long search for chromate replacement in corrosion protection.² Despite intensive research efforts, both academic and industrial, the sunset date is repeatedly prolonged for various applications, with the flagship being the aerospace industry. A quick literature survey will lead to thousands of publications presenting new alloys, coatings, or corrosion inhibitors as the next technological breakthrough. The Valley of Death is full of compounds, formulations, and data worth billions of dollars as well as an unthinkable number of person hours. We believe that this is a result of how we do exploratory research in general and holds for many other fields such as alloy research, electrocatalysts,³ or composite materials⁴ due to a multitude of reasons, including the following:

- Research is performed in a disconnected way; FAIR⁵ data principles are not followed.
- Classical experiment reporting leads to anecdotal success stories rather than real breakthroughs, and there are limited data regarding what has been previously tried but was unsuccessful.
- Research focuses on minor modifications to established materials.
- Correlations presume subjective criteria, lack causality, and are superficially generated.
- Results obtained at small-laboratory scale cannot be translated to application.

As a response to the recent call “Reaching critical MASS (materials acceleration for societal solutions),”⁶ this white paper presents our ongoing commitment to establishing a joint Canadian-German materials acceleration platform (MAP) aimed at the discovery of next-generation structural and functional materials with a focus on durability, sustainability, and economic feasibility. We call our idea the “Build to Last Materials Acceleration Platform” (B2L-MAP). Briefly summarized, it is a multi-level platform that goes beyond lead generation by integrating upscaling, technical feasibility, and durability/corrosion analysis of the leads via smart proxy experimentation. Moreover, the lifetime CO₂-footprint calculation, material availability assessment, and cost analysis will be incorporated into lead generation in addition to the performance-based ranking to enable researchers to freely reconfigure the weighting criteria to meet their material design specifications. Thus, through consideration for the locality of available energy types and critical minerals resources, even for the same starting materials, German and Canadian B2L-MAPs or spin-off MAPs all around the world will be able to operate with different parameter space boundaries. The output of the B2L-MAPs will be Pareto optimal alloys that balance performance, maximize CO₂ neutrality, and minimize the use of critical minerals. We believe that the B2L-MAP idea has the potential to not only generate material libraries connecting performance descriptors with durability descriptors but also to take the first steps toward using such libraries to find substitution solutions that secure material availability for the coming decades.

NEW ALLOYS AS ENABLERS OF CLEAN ENERGY TRANSITION

For the rollout of the B2L-MAP, we set our eyes on one of the harshest environments on this planet and a system that will be a key enabler of the clean energy transition. With the versatility of use cases ranging from electrification of heavy-duty vehicles and maritime transport to the production of green steel, hydrogen will be the future energy carrier to enable global energy security and accelerate decarbonization of

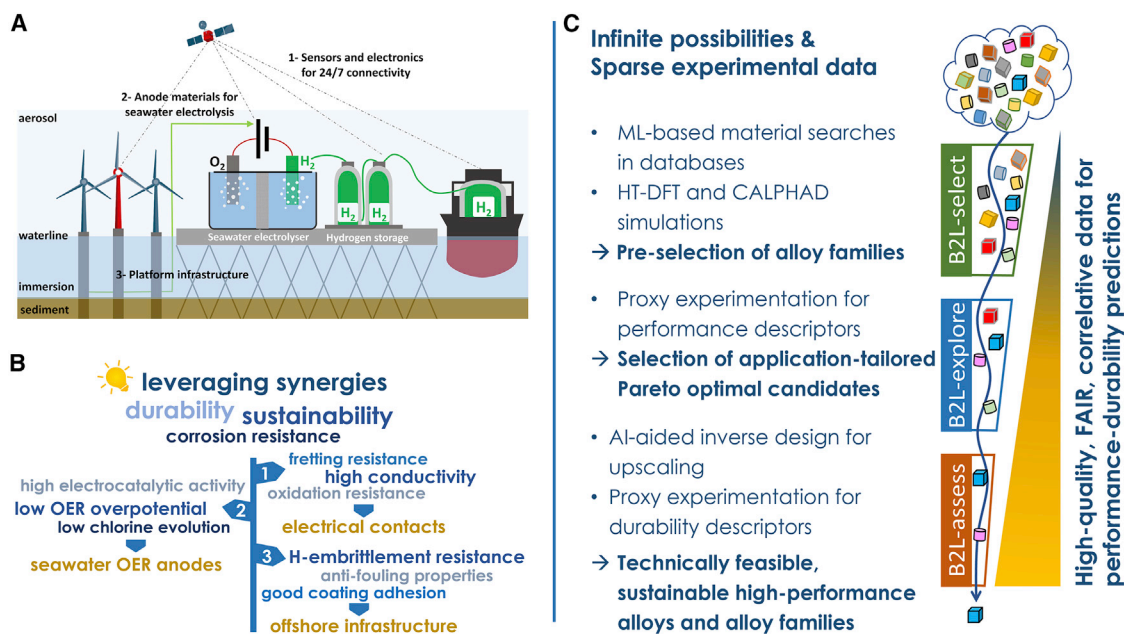


Figure 1. Vision of B2L-MAP

(A) Three envisaged material challenges of B2L-MAPs as enablers of the safe operation of an offshore wind farm dedicated to hydrogen production.

(B) B2L concept to leverage synergies in exploration with differential material optimization for three challenges.

(C) Three-tiered structure of the B2L-MAPs.

heavy industries. Thus, we urgently need to explore technologies and materials that will enable efficient, local, and sustainable production of hydrogen. Moreover, the societal acceptance of hydrogen technologies will depend significantly on the safety and durability of this infrastructure, meaning that we must build them “right the first time.”⁷

Motivated by this challenge, B2L-MAPs will develop next-generation alloys for addressing three main material-related challenges associated with realizing an offshore wind farm dedicated to hydrogen production. Recent modeling studies by Dinh et al.⁸ and Bonacina et al.⁹ demonstrated that a dedicated offshore wind farm for hydrogen production would be profitable by 2030 for a wide range of scenarios and could also offer solutions to meet the environmental targets of the maritime sector with new on-route refueling possibilities. Such a self-sustaining offshore installation (Figure 1A) will ideally be remotely monitored with a plethora of sensors and will need fail-proof connectivity.¹⁰ The electrolyzers would ideally operate on seawater directly without energy-intensive desalination treatments to maximize energy efficiency.¹¹ Finally, the critical infrastructure must be corrosion proof and resistant to hydrogen embrittlement, especially under cathodic corrosion protection conditions.¹²

The common denominator between durable electrical/sensor hardware (B2L-challenge 1), electrolyser oxygen evolution reaction (OER) anodes (B2L-challenge 2), and offshore infrastructure (B2L-challenge 3) is that they all are components whose success relies upon the development of novel, sustainable, and economically feasible alloys with excellent durability. Utilizing the limitless multi-dimensional compositional space that multi-principal element alloys (MPEAs) offer, B2L-MAPs will aim to use the strengths of artificial intelligence (AI)-driven materials discovery and high-throughput experimentation to identify new MPEA families.

Previous work within the MPEA space has demonstrated the reason for optimism. Superior corrosion resistance and lower onset potentials for the OER were reported for CrCoNi¹³ and CrCoMo¹⁴ alloys, qualifying them as potential anode materials in addition to more classical applications as structural or implant materials. In the related field of metallic glasses, a combination of a machine-learning (ML) model and high-throughput experimentation was demonstrated as a means of rapidly identifying new alloys with superior mechanical properties.¹⁵ Rao et al. recently applied a closed-loop, integrating ML approach using density functional theory simulations, thermodynamic calculations, and experimental validation. They were able to narrow down the composition space of high entropy Invar alloys with extremely low thermal expansion coefficients to 17 out of millions of possibilities by ML-assisted simulations and to two candidates after experimental validation.¹⁶ Moreover, excellent mechanical properties and wear resistance were reported with thermal spray MPEA coatings even before the term high-entropy alloys (HEAs) became en vogue.¹⁷ The known segregation behavior of Cu in fcc-MPEAs into interdendritic regions¹⁸ can be utilized effectively to generate materials possessing high conductivity pathways in bulk alloys that retain the superior mechanical properties associated with the MPEA solid-solution phase.

Briefly summarized, when it comes to alloy development, we believe that the periodic table is still full of possibilities and that making alloys is more than just combining the elements together. The pre-MAP era has discovered some very reasonable points of this multi-dimensional parameter space and generated a solid knowledge basis of basic mechanisms as well as excellent tools for advanced characterization. The B2L-MAPs will build on this expertise by combining the available computational and experimental tools, devising new efficient proxy experiments for performance and durability assessment, and harnessing AI-guided efficient exploration. This unprecedented amount of knowledge generated in terms of structure-property/environment-durability correlations will lead to the discovery of entirely new alloy families. The exploration for the selected extremely harsh offshore environment will be primarily a simulation-aided bottom-up approach. However, as the B2L-MAPs and its material libraries mature, top-down material searches for applications with lower corrosion loads would easily be possible and lead to spin-off successes in material substitution for a wide range of applications.

CONCEPT OF THE B2L-MAP

B2L-MAPs will be built to accommodate an AI-driven active-learning approach to discovery, as shown in Figure 1C. The B2L-MAP runs in a three-mode low-fidelity to high-fidelity system, utilizing computational tools for alloy knowledge generation and selection (B2L-select), a low-latency exploration platform for efficient lab-scale assessment (B2L-explore), and a higher-latency scale-up platform for industrial applications (B2L-assess). AI will link the three platforms for recursive feedback of knowledge generation, ultimately driving transferability between computational, lab-scale, and industrial-scale performance. In Figure 2, the three modes of this approach are summarized.

B2L-select will develop ML models to act as surrogates to computational data for the purpose of selecting and screening families of alloys. Active learning will drive the computational materials science simulations to efficiently generate data and knowledge models. Simulations will be realized predominantly via parameter-free high-throughput density functional theory (HT-DFT) calculations, which are routinely used to explore the experimentally uncharted materials space.^{19–21} The existing

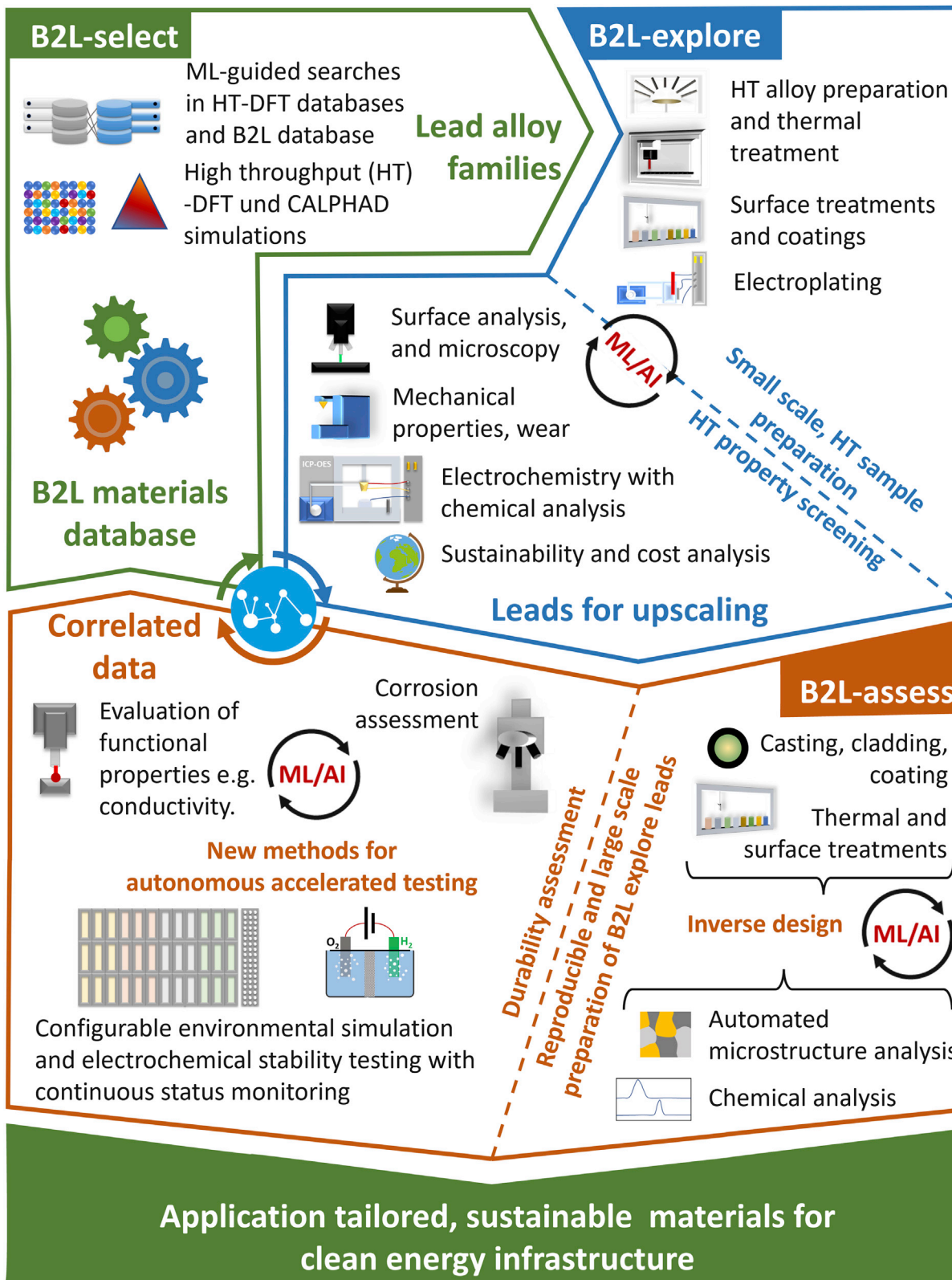


Figure 2. Concept of the B2L-MAP

B2L-MAP will perform AI-guided, close-loop material design campaigns with autonomous workflows starting with simulation-aided pre-selection (B2L-select) followed by lead generation (B2L-explore) and upscaling/technology assessment (B2L-assess).

large HT-DFT databases (e.g., Materials Project, AFLOW, OQMD) and on-demand HT-DFT calculations will be leveraged to train ML models, with physical features extracted from chemical formula or from atomic structures,²² for efficient pre-screening based on, e.g., Pourbaix diagrams^{23,24} and elastic properties.²¹ These ML models trained with both computational and iteratively acquired experimental inputs have a great potential to improve accuracy compared with the ones trained with only experimental data.^{15,25} In addition, empirical modeling such as CALPHAD shall also be employed for HT screening,²⁶ especially for the search for composition spaces containing single-phase MPEAs. If necessary, kinetic models such as molecular dynamics or phase-field crystal at the atomic level, phase field at the mesoscale, and finite-element-based models at the macroscale could later be implemented to aid in the transition from B2L-explore to B2L-assess, tying chemistry-structure relationships to determine methodology and feasibility of scale up. These simulations will be linked to the data and task management platform and ML models to efficiently explore the alloy-property parameter space.

B2L-explore performs lab-scale experiments in the regions of materials space identified by B2L-select, integrating common electrochemical hardware into a single AI-driven synthesis and characterization platform. This platform will support material preparation and chemical/electrochemical surface treatments. Moreover, techniques for analyzing surface chemistry and electrochemical properties as well as assessing the surface morphology and wear resistance will be integrated into the workflow. Active-learning systems will be utilized to generate models relating physical parameters and to efficiently explore the parameter space by guiding the next iteration of the exploration.¹⁶ At the lowest level, Gaussian process regression and classification will be employed to create efficient mapping strategies that permit the acquisition of a full phase-corrosion resistance/catalytic activity/wear-resistance diagram from each library without the need to redeposit a new film. At the highest level, correlations and newly discovered physical linkages between the measured properties will permit sparse sampling of time-consuming measurements/processes by using rapid measurements of a property (say, corrosion resistance/durability) to inform the posterior distributions of other properties (e.g., phase composition). This is premised on discovering and quantifying the interrelationship between composition, processing, and properties over as broad a range of alloy-electrolyte chemistries as possible. For instance, thin-film physical vapor deposition (PVD) tools will be used to prepare combinatorial libraries that cover full three-, four-, or five-component systems in a single deposition.²⁷ Similarly, high-throughput alloy synthesis via radio frequency inductively coupled plasma has recently been demonstrated to produce as many as 32 samples in parallel.²⁸ The characterization of crystal structure (X-ray diffraction [XRD]), composition (X-ray fluorescence [XRF]), corrosion resistance, catalytic activity, and wear resistance will be accomplished via integrating existing autonomous capabilities into a single connected workflow. The inherently multi-modal nature of this problem and the expected underlying connections between composition, phase, and performance will create opportunities to provide comprehensive understanding of the full spectrum of properties tested. Within 2 years of full platform operation, B2L-explore will be able to create a massive dataset containing more than 50,000 composition/processing/structure/multi-modal-property measurements of previously unexplored materials and a set of science-informed AI models capable of predicting the properties of millions more alloys with a quantification of their uncertainty.

B2L-assess will down-select the alloys provided as leads by B2L-explore for upscaling via inverse design and for in-depth testing based on their projected ability to satisfy the durability requirements of one or more of the three technological pillars. An inverse design approach will be necessary as the leads of B2L-explore will be generated on the basis of small-scale samples, often with compositional gradients. The synthesis goal of B2L-assess will be to use inverse design in given compositional spaces to achieve the same property descriptor values reproducibly in a given confidence level on large-scale samples with statistical validation. The second focus will be in the automation of durability testing. These will include environmental simulations such as salt aerosol, aqueous immersion, sediment immersion, thermal cycling under controlled humidity, and various electrochemical tests depending on the targeted application. It is a well-known fact that standardized testing methods such as the neutral salt spray test come up short when it comes to reproducing the types of corrosion in automotive applications and have difficulties in predicting the durability of automotive products.²⁹ Furthermore, electrocatalysis durability studies (e.g., OER) require extended test times, even with the inclusion of accelerated stress-testing protocols, and new approaches need to be developed through both advanced characterization techniques as well as simulation and/or AI-assisted predictive models to reduce the time for evaluation. In the MAP era, new tools for parallelized accelerated testing will be necessary, which go well beyond determination of pitting potentials and dissolution quantification paradigms and extend to a holistic understanding of durability of functional materials. Thus, the B2L-assess will devise and validate new proxy durability experiments that are application tailored. An ML-based approach will be applied for the in-depth analysis of the B2L-assess test data with the aim to explore correlations that are not identifiable by human inspection or traditional statistical analyses. This serves the overarching aim of developing self-learning testing methods as AI-guided sampling can increase the efficiency of durability evaluation significantly and thus accelerate the bench-to-market transition.

The major risk in designing a MAP for the discovery of corrosion-resistant materials is that it must handle complex metallurgical and other preparatory processes such as alloy synthesis, metal film deposition, or thermal treatment. Moreover, upscaling of synthesis and post-treatment steps is not a trivial task and will require AI-aided guidance. As upscaling and technical feasibility are major bottlenecks in the material innovation chain and one of the reasons behind the commercialization Valley of Death, these challenges must be tackled in this concentrated atoms-to-turbines effort to ensure effective stewardship of technologies into application.

B2L-MAPs in Canada and Germany will follow two different paths to address this issue. While the Canadian B2L-MAP will be supported by multi-target gradient PVD, select alloy casting and thermal treatment, and electrodeposition for the alloy synthesis, the German B2L-MAP will focus on high-throughput alloy development via arc-melting and laser-based local thermal treatments. This branching will not only enable effective risk mitigation but also significantly enhance the complementary nature of the collaboration as well as the depth of the generated material libraries. Moreover, the synthesis methods will benefit from the modules of MAPs and related activities currently in progress at consortium partners (e.g., TEG-MAP @NRCan-Hamilton, MatSpace@BAM), creating synergies and lowering the investment budget of the projects. Due to the long sample preparation and processing times, the ML algorithms in the explore level will be designed to operate flexibly either in one-sample-at-a-time mode or in high-throughput batch mode, which would be necessary for alloy and gradient film synthesis.

To allow a direct link between the explore and assess levels, the B2L-MAPs will follow a sample-centric design that generates a semi-structured, interchangeable data thread for each sample that will contain raw and processed data together with the metadata and platform status monitoring information. This data management will be structured based on operational flow, such as the systems built at University of Toronto³⁰ and archival/data sharing systems currently being built at NRCan, or leveraged from open-source platforms such as MDCS or Materials Commons.^{31,32} Beyond these structured approaches available for dealing with agnostic data exchanges between components, in B2L, framework-specific data structures will be established for non-agnostic usage at the exchange endpoints as well as workflow identification and implementation. The findability of the datasets in the archive will require a searchable archive system, allowing both manual and automated search algorithms using data labels and tags.

The desire to break from the status quo “copious amounts of data with a lack of detailed description and information” is the driving force behind the ontology work. Missing information is the bottleneck on the path from data to key findings that can be used to generate knowledge that will have long-lasting impacts. This will be one of the priorities of the B2L-MAPs, especially because the goal of combining the long-term performance data with the property descriptors evaluated with simulation or lead-generation experiments requires automating as much as possible of the detailed bookkeeping for each and every sample. This is the one aspect that will make the B2L-MAP concept rise or fall.

Full-scope B2L-MAPs are expected to be progressively developed over a term of 5 years with an overall budget of \$10 million USD equally shared between the Canadian and German partners. The long-term strategy is to integrate the B2L-MAPs into the bigger MAP competence centers currently in the planning phase in Canada and Germany. These user facilities will offer project-based access to B2L-MAPs for academic and industrial partners, with adapted data policies and a special focus on supporting small and medium enterprises in their innovation processes.

ADDED VALUE OF B2L-MAP FOR THE MAP COMMUNITY AND SYNERGIES WITH OTHER INITIATIVES

The B2L-MAP will operate at the crossroads between digitalizing a highly conservative discipline and materializing abstract concepts such as performance and stability descriptors to create a fundamental understanding of the underlying science. As recently demonstrated by Umehara et al.,³³ we believe that the real discovery path from data to result, from result to key finding, and lastly from key finding to the mechanistic understanding is only complete with human interpretation. Thus, we will follow an “all-hands-on-deck” principle and will make the non-proprietary platform data available real time during the development phase for further use.

Developing the necessary hardware and disseminating the necessary software tools for the realization of B2L-MAPs will significantly advance the interoperability of MAPs around the world. The core of the platform, the three-tiered AI backbone, as well as the data structure will be jointly developed by teams from Canada and Germany. As it is common with many MAP concepts, the B2L will be a material agnostic MAP and can easily be reconfigured to investigate other scientific questions from the surface/electrochemistry/functional materials fields. The data platform will be built on a modular data agnostic transfer and storage system to facilitate data transfer between disparate operations. The transfer system is agnostic to the

specifics of the data, leaning on the specific systems to understand the standard formatting for its operations while capturing metadata tags to identify needed material and property specificity in longer-term archival storage for future utilization. This allows a common system to be utilized for any number of MAPs systems while still retaining material specificity to search and combine in optimization or exploration goals. Though highly interoperable, the data structures and systems will provide for secure transfers that enable confidential or proprietary work as well as providing open access when for the public good. Adaptation of the B2L-assess concept and tools to other MAPs have the potential to push the innovations in other fields from the exploratory stage to higher technology-readiness levels (TRLs). Moreover, quality management processes are very rapidly digitalizing, and the trend goes in the direction of process validation and will eventually phase out the classical sampling-based quality control approaches. The MAPs will conceptually contribute to this process by creating a gapless sample record like a blockchain.

The inclusion of the long-term property evaluation, reproducibility check, and stability analysis with the B2L-assess level will increase the scientific trust in AI by objectively challenging our simulation capabilities, AI concepts, descriptor selections, and pseudo-experiment designs. Together with the real-time open-data commitment and pro-active outreach work, we believe that B2L will be a testbed for fully autonomous materials discovery reaching TRLs 4 to 5. Moreover, the material systems under investigation will be tied closely to downstream integrators that can move the technology to higher TRLs and, ultimately, commercialization. Furthermore, the trust in AI can profit significantly from the transition of AI-enabled key findings into human-generated fundamental knowledge that profits equally from the best of the two worlds.

The development of MAPs can only be tackled with a convergence approach. Considering the details of the B2L-MAP, complex metallurgical and preparatory steps, as well as the surface analysis and electrochemical tools planned for integration, the joint efforts of material scientists, chemists, and physicists supported by mechanical engineers, robotics, and mechatronics experts as well as programmers and data scientists will be needed. These multi-disciplinary teams are already under development in select government and academic laboratories, which will accelerate the implementation of the B2L-MAP platform. B2L-MAPs will profit significantly from the MAPs in Canada (EMAP @NRC-Mississauga, TEG-MAP @NRCan-Hamilton) and Germany (FRIDA @BAM) that are currently in progress. The major investment by the Canadian government to build a center for accelerated materials discovery and innovation at the NRC-Mississauga site has great promise to advance this important global issue. The fascinating role of MAPs in the educational space, especially in natural sciences and materials science, is that the ongoing activities around MAPs will make the boundaries between these disciplines more fluid.

The creation of end-to-end innovation processes requires that production steps be fully automated, which is already largely established in related industries. The scale up and durability testing in B2L-assess is the necessary step to go from early-stage discovery to technology validation in relevant environments (TRL 5). Beyond this point, collaborations in exploratory projects will transition to consultancy during the pilot phase at industrial research and development (R&D) facilities. Both teams are working for the establishment of an industrial advisory board in cooperation with NRC-IRAP (Canada) and AiF (Germany) to integrate the industrial stakeholders, especially from the small- and mid-size enterprise (SME) sector, as early as possible in the B2L development.

Demand for knowledge and data about corrosion and durability is growing as they are necessary to enable the development of technologies to harness alternative energies such as solar, wind, hydrogen, and biomass. These applications often involve exposing the engineering structures and components to highly hostile environments. On one hand, with increasing technological advances, there is a need to develop high-performance alloys and materials, in particular intrinsically corrosion-resistant materials. On the other hand, with the advent of new materials processing and manufacturing technologies such as additive manufacturing, we need to understand the corrosion behavior of materials manufactured through these emerging technologies and routes. A lack of corrosion knowledge and data hinders our ability to design new materials with desired performance and to prevent disastrous failures.

The development of B2L-MAP will provide us with powerful tools and generate knowledge and data to address the four grand challenges of corrosion³⁴ for the corrosion research community and industrial users: (1) development of cost-effective, environment-friendly, corrosion-resistant materials and coatings; (2) high-fidelity modeling for the prediction of corrosion degradation in actual service environments; (3) accelerated corrosion testing under controlled laboratory conditions that quantitatively correlates with observed long-term behavior in service environments; and (4) accurate forecasting of remaining service time until major repair, replacement, or overhaul becomes necessary (i.e., corrosion prognosis).

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AUTHOR CONTRIBUTIONS

Conceptualization, writing – original draft, and writing – review & editing, all authors.

DECLARATION OF INTERESTS

J.H.-S. was involved in ideating and soliciting papers for the special collection that this work is a part of.

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