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Explainable Graph Neural Network Framework for Multi-Objective Discovery of Next-Generation Battery Materials Using Limited Experimental Data

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Abstract

Exploring the vast chemical design space to find better electrode and electrolyte materials is a roadblock to electric mobility and grid scale storage as no laboratory can keep up. While graph neural networks (GNNs) are a promising method for estimating material properties from the atomic structure, limited use of GNNs in battery research is due to three limitations: predictions from GNNs are hard to interpret, they are typically trained for a single target, and they require labelled data which is limited for new chemistries. This paper provides a review of recent research on graph-based learning, explainable artificial intelligence (XAI), data-efficient learning and multi-objective optimisation for battery materials discovery focusing on eight key studies alongside supporting examples from the last five years (2021–2026). literature. It can be seen from the criterion-based comparison made that no single of the reviewed studies covers the topic of representation of the graph, Explainability, multi-objective trade-offs, limited-data learning and experimental validation. Filled with this need, we We provide a well-defined conceptual framework for graph construction, uncertainty-aware GNN prediction, explanation, Pareto-based candidate selection and DFT/experimental verification, and define an evaluation protocol for it. The framework is suggested rather than applied and open challenges and future directions are discussed.

Keywords: Battery materials, Explainable AI, Graph Neural Networks, Limited Data Learning, Materials Informatics, Multi-Objective Optimisation, Voltage Prediction.

I. Introduction

Lithium-ion batteries and newer, sodium-ion batteries. Underpin electric, underpin multivalent-ion, and solid-state designs. vehicles, portable electronics and the storage needed for intermittent renewable power. Requirements in terms of energy density, satisfies the criteria of safety, service life and cost, which are continually improving. calls for new electrode and electrolyte materials. The classical approach to such materials is to alternate synthesis and. Lab characterization of the characterization. Each iteration is slow and costly, while the number of possible compositions and crystal The combinatorial size of structures is enormous [1], [2].

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The plants are developed before any synthesis is created. Since crystals and atoms and the bonds between atoms are the natural description of molecules. between them, graph neural networks can learn from this structure directly. A graph convolutional network is used to create crystals [3] and Material's Graph Networks (MEGNet) [4] were early demonstrations, large-scale GNN-guided exploration has Including extra, larger crystals [5], since enlarged the set of known stable crystals To filter out high voltage levels, regressors of average voltage have been used. voltage sodium cathodes [6].

Nevertheless, there are three limitations for practical battery research. First, most GNNs are blackboxes, that is, a research scientist must rely on their external behavior. can't identify the atoms, bonds or descriptors that are responsible for a However, an interpretable design is beginning to be developed (prediction). appear [7], [8]. Secondly, there are several equilibrium equations to consider in a real cell. competing properties, most models are tuned for. one. Third, there are labelled data available for new chemistries, which has sparked few-shot and zero-shot strategies, smalls [9].

This paper makes the following contributions.

- Review and outline of recent research on GNNs, XAI, limited data learning and multi-objective battery materials.
- An alternative solution to the problem to the one that is already developed. Conceptual, end-to-end framework that brings together the 4 themes; proposed evaluation protocol.
- A discussion of applications, limitations and future directions.

The rest of the paper is organised as follows. The background is presented in Section II, literature is reviewed in Section III, research gaps are discussed in Section IV, the framework is presented in Section V, applications, limitations, future work and conclusions are presented in Sections VI–IX.

II. Background

A graph is used to represent materials are represented by a graph. A material is a graph $G = (V, E)$, with a node v corresponding to an atom and a node on the edge e_{uv} corresponding to a bond, or a pair of neighbouring atoms within a given cut-off distance. The attributes of the nodes are typically the atomic number; the attributes of the edges typically are the interatomic distance (or bond type); and the attributes of the nodes are typically electronegativity, ionic radius and valence. Neighbours are searched over periodic images of the unit cell for crystals. Structures (and computed properties) that can be converted to graphs in this way can be obtained from open databases, such as Materials Project [10].

A. GNN-Based Property Prediction

Most frequently used material of GNNs is based on the message passing scheme. Each node receives from its neighbouring nodes at layer l, and keeps updating its hidden state:

$$h_v^{(l+1)} = \varphi\left(h_v^{(l)}, \oplus_{u\in \mathrm{N}(v)} \psi\left(h_v^{(l)}, h_u^{(l)}, e_{uv}\right)\right) \quad (1)$$

The permutation-invariant, which constructs messages, is the one that you are familiar with. The update function is denoted by φ and the aggregator is either the sum, the mean or the max. At the end of L layers a readout collects the states from nodes into a graph level vector which is input to a prediction head:

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$$\hat{y} = \rho\left(\oplus_{v \in V} h_v^{(L)}\right) \quad (2)$$

B. Explainable Artificial Intelligence (XAI) for Graph Models

Two general kinds of explanation methods exist: Post-hoc methods involve studying a trained model, such as GNNExplainer [11] that looks for a small subgraph and feature mask which will preserve the prediction of the model. Intrinsically interpretable designs lead to adding transparency to the architecture, such as, these are done by using attention weights [7] or additive structures [14]. Explanation are typically evaluated based on fidelity (does the explanation adhere to the text? Is it readable (explanation) and is it compact enough (or sparse enough, sparsity)? A multi-objective search approach might be able to improve both at the same time [8].

C. Learning from Limited Data

The following approaches, which reduce the amount of labelled samples required, have been considered: pre-training on a large set of computed samples and fine-tuning, transfer of learning between similar properties, few-shot learning, zero-shot inference using material embeddings [9] and active learning to select the most informative samples for labeling and physical knowledge as priors or constraints.

D. Multi-Objective Optimisation

The design task will be transformed into a problem that has k objectives.

$$\min_{x \in X} F(x) = [f_1(x), \ldots, f_k(x)] \quad (3)$$

Let x_a and x_b be two candidates. x_a is said to dominate x_b if and only if $f_i(x_a) < f_i(x_b)$ for some i and equal to for all i. The non-dominated candidates are presented as the Pareto front, where the decision maker is given all the trade-offs instead of just a weighted score. The evolutionary algorithms that are used are NSGA-II. Evolutionary algorithms (NSGA-II) are employed. There are many methods available to approximate this front, one of which uses [12] to do so.

III. Literature Review

The type of method, main result of the study and limitations described by the authors of the 8 primary studies were analyzed. Table 1 summarizes this information.

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Table 1: Summary of the Reviewed Studies

Ref. / Year	Approach and main finding	Reported limitations
[13] 2026	The Graph representation the Learning of Linked data is a crucial step. cathode microstructure; and outperform the image-based in predicting performance.	High compute cost; needs high-resolution 3-D imaging; little industrial validation.
[1] 2025	Learn the about 2025 perspective on ML paradigms, For battery science , for ML; speed up discovery, manufacturing and management.	Scarce data; weak generalisation; uncertainty; scale-up; experimental checks.
[7] 2025	Readable decisions for improved structural classification; interpretable GNN with attention.	Trade-off: interpretability vs. accuracy; scaling of large-graphs; complexity.
[2] 2025	Acceleration of discovery through DFT + ML screening of high entropy materials.	The search space is large, the DFT is expensive, and there are not many benchmarks.
[14] 2024	Explainable neural network (GAM-SI) – sensitivity analysis; ranks the parameters of the process which affect the electrode loading and porosity.	Very noisy factory data, restricted real-time use, high amount of sensor uncertainty.
[9] 2024	Zero-shot learning using material embeddings; discovers the label-less, promising organic battery materials for each class.	Domain shift, sparse labels, reliability, lab confirmation.
[15] 2022	Interpretable ML for electrode voltage; reveals chemically meaningful descriptors.	Limited data diversity, accuracy vs interpretation, physics integration.
[8] 2021	Multi-objective explanation of GNN predictions; more faithful and compact than single-objective explainers.	Optimisation the complexity; overhead; consistency; and scalability..

Graph-based learning. Li et al. [13] show that representing a Connectivity effects can be captured by the cathode microstructure as a graph. While models based on pixels are missing, the approach depends on. costly 3-D imaging. Joseph et al. [7] combine an attention mechanism with GNNs. To acquire structure classifications that can be inspected, while Recognizing that some loss of accuracy may be incurred in the process of making the model interpretable. At the largest scale, GNN-driven discovery has produced millions The voltage regressors are the same ones used in the regression of electrode voltage [6] and the candidate crystals [5]. Sodium cathodes have been used with based on GNNs [6].

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Interpretable data-driven models. Liu et al. [14] use an The ADDIE model is used to identify which production. The parameters control the mass loading and porosity of the electrodes, Zhang et al. [15] address this issue by extracting chemically meaningful descriptors. For multivalent-ion electrolytes, predicting the voltage. Both exemplify two ways to achieve transparency, but neither of them works. on atomistic graphs. Liu et al. [8] come closest to graph problem that is broken down into several objectives.explanation as a multi-objective problem is broken down into several objectives. problem.

Small amounts of data, large amounts of simulation. Wang [1] argues that When designing applications using ML, small datasets must be dealt with, uncertainty and verification. This, in turn, is the reason why Park et al. [9] chose to develop a new device. The task of a seemingly zero-shot inference on material embeddings Is labeled with each material class. However, Mashhadimoslem et al. [2] use DFT and ML to study But some of them sacrifice accuracy for simplicity of computation, in the form of high-entropy materials. cost.

IV. Research Gap Analysis

All of the reviewed studies were marked up with a view to making the gaps clear. This article will be expressed in terms of five criteria: graph representation, explainability, multi-objective treatment, few data learning and experimental are some of the most crucial research challenges. validation. The rating in the Fig. 1 is the authors' qualitative rating. The results of these studies summarized in tabular form (Table 1) is not a quantitative representation of the findings of the studies. tative benchmark.

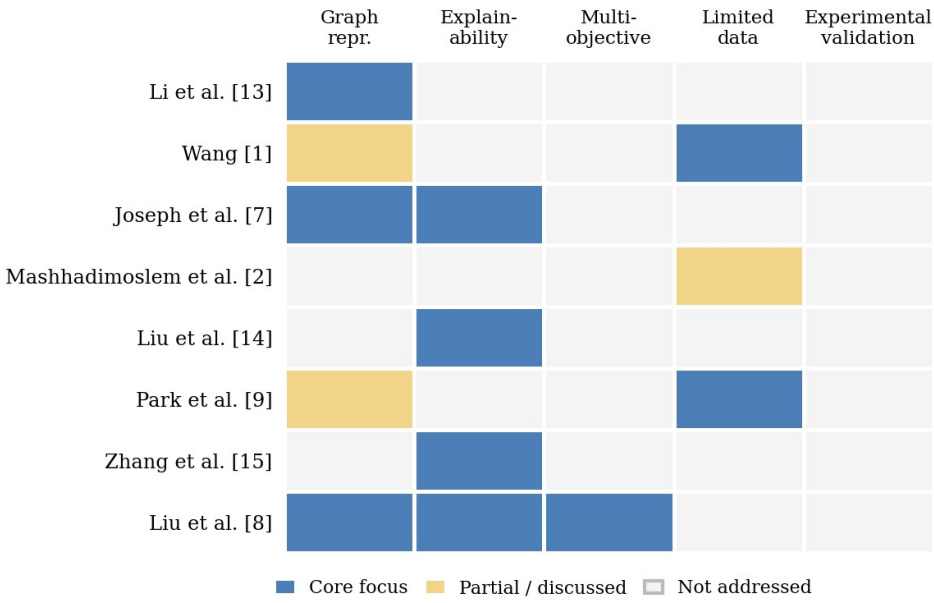


Fig. 1. Coverage of five design criteria by the reviewed studies (qualitative rating).

The following can be seen from the matrix:

- **G1 – Opacity.** A number of models of graphs provide little insight into For what reasons materials may be successful.

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- **G2 – Single-target focus.** This is only taken into account by one study [8]. where there are multiple objectives, it is an explanation, Not the Battery characteristics.
- **G3 – Data limits.** A good experimental data is scarce – decreases accuracy, decreases generalisation.
- **G4 – Fragmentation.** To the best of our knowledge, there is not yet a study that integrates GNNs and XAI. One pipeline for and multi-objective optimisation.
- **G5 – Verification.** The following is an experimented confirmation of AI-: Rarely is a reference ever made to the reporting of proposed candidates.

V. The Envisioned Conceptual Structure

To obtain a solution for G1–G5 we proceeded to sketch the pipeline in: There is no introduction or standardisation, The results of these experiments are presented.

A. Construction of Data and Graphs

The input is a composition and structure that comes from the public. Data repositories [10] and in-house measurements (where available). Structures are transformed to graphs as outlined in Section II. A small but trusted experimental group is set aside as a “holdout” group set that is not ever employed for training.

B. Data-Driven GNN Predictor

A GNN encoder is pre-trained with a lot of computed data properties and then fine-tuned on the few experimental labels. Few-shot or zero-shot components can be used for chemistries. It includes nearly no labels. Several prediction heads guess the voltage, capacity, stability and related targets and ensemble or Monte-Carlo dropout gives an estimate of the uncertainty in every output to indicate if a prediction is unreliable.

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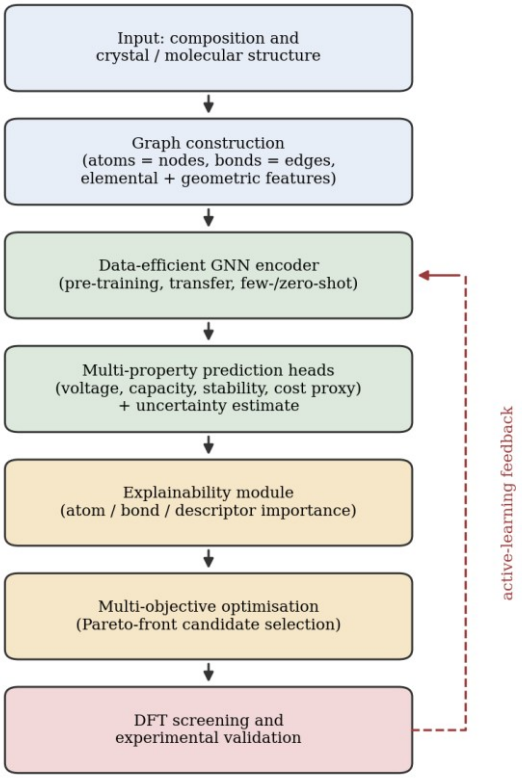


Fig. 2. Proposed explainable, data-efficient, multi-objective discovery pipeline.

C. Explanation Layer

For each prediction, a subgraph mask like that of a GNNExplainer. The atoms, bonds are highlighted in [11] and descriptor attribution [15] respectively. and includes important attributes. The quality of explanations is continued in line with [8] as follows: Was viewed as a compromise between fidelity and sparsity. Chemists can then verify that there is agreement between the highlighted substructures Known chemistry that serves as a sanity check of the model.

D. Multi-Objective Candidate Selection

The properties predicted are correlated to the objectives in Table 2. and was passed to an evolutionary optimiser (NSGA-II) [12]. The result is a Pareto front, which is shown in the concept of Fig. 3. The domain experts select from Fig. 3 on the basis of. application.

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Table 2: Candidate Objectives and Proxies

Objective	Candidate proxy	Direction
Energy density	Expected mean voltage × specific capacity	Maximize
Optimize Stability	Formation energy / energy above hull	Maximize
Optimize Safety	Indicator of Structural and thermal stability	Maximize
Optimize Cycle life	Volume change during (de)intercalation	Minimize
Cost	Abundance of elements / price proxy	Minimize

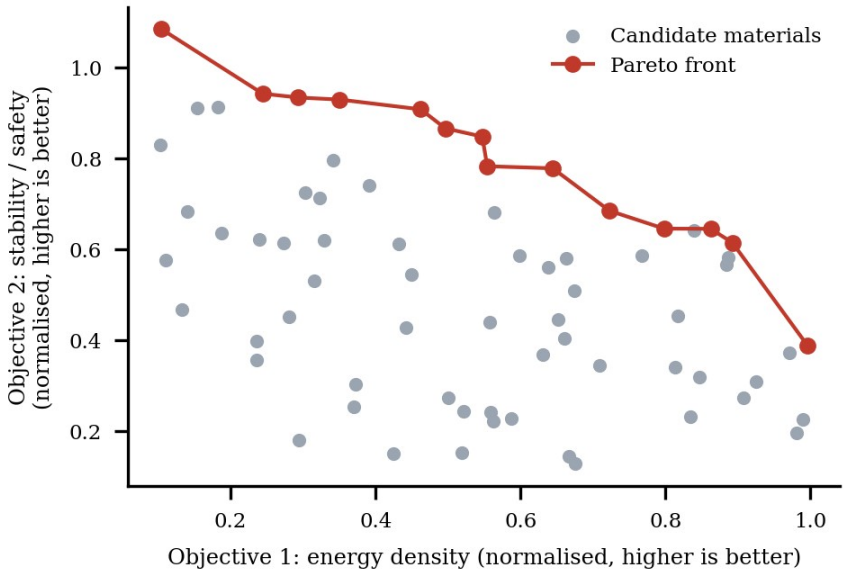


Fig. 3. Conceptual Pareto front for two objectives (schematic illustration with synthetic points, not experimental data).

E. Validation and Feedback

Candidates who make it to the short-list stage are then subjected to DFT verification of stability. and voltage, and the most promising are passed on for lab-, however further testing is still required. oratory synthesis. The measured outcomes are brought back to the training. make and control the next set of candidates to be examined, an active-learning loop.

F. Evaluation Protocol

The three-step framework should be compared to appropriate baseline(s), Such as a conventional GNN without explanation or multi- Using objective stages and a regressor based on descriptive characteristics. The measures listed in Table 3.

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Table 3: Proposed Evaluation Metrics

Component	Metrics
Property prediction	MAE, RMSE, R^2 on held-out and low-data splits
Uncertainty	Calibration error; error–uncertainty correlation
Explanation	Fidelity, sparsity, stability across random seeds
Optimisation	Hypervolume, spread of the Pareto front
Validation	DFT agreement; fraction of candidates confirmed in the lab

VI. Applications

When realised, the approach can help with the development of tems, and e-mobility solutions. Electric vehicle, renewable energy storage systems and e-mobility solutions. Testing of solid state batteries; research into solid state batteries. and simulation screening of novel chemistries (for) There is a limited amount of labelled data available. Since explanations refer to struc- The output can also inspire experimentalists in the development of tural motifs. chemically sensible modifications.

VII. Limitations and Challenges

The review can only include a few primary studies, so conclusions about the literature as a whole should be drawn from these. Should be considered with care. With the proposed framework, There are several significant challenges, such as the availability of accurate Experimentally tested data, training costs of GNN and DFT validation error The following will be addressed: tion, prediction uncertainty, distribution shift between training and test time, and model uncertainty. New materials and real new ones, the scalability of graph, models, potential omissions of explanations, or misleading, and necessary laboratory confir- The term predicted candidates refers to those that the student has made himself.

VIII. Future Directions

Much promise lies in the extensions to GNN architecture, such as the physics-informed GNN. The last three presentations focused on 3D printer printing materials, transfer learning between chemistries and greater few- scenario analysis are employed. shot and zero-shot methods, uncertainty-aware prediction, and scenario analysis are used. Active learning with experiments that completes the loop. Tighter coupling of machine learning with simulation and automated Further research into experimentation should enhance reliability. Implementing and benchmarking the proposed framework on public battery datasets is the natural next step.

IX. Conclusion

Recent advances in graph-based, explainable artificial intelligence (XAI) for network analysis and spatio-temporal forecasting are reviewed here. Battery able, data efficient and multi-objective learning However, there are no studies that combine all of the materials, and showed that no single study does. These elements were validated by experiments. We proposed a It is conceptual framework and evaluation protocol that bring together the concepts in the program. them together. Such an approach might make AI-assisted drafting a win-win scenario. It is, however, more transparent and more economical to discover battery

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materials. in data, and better matched to real design trade-offs, provided. in which it has been confirmed by simulation and experiment.

References

[1] Y. Wang, "Application-oriented design of machine learning paradigms for battery science," *npj Comput. Mater.*, vol. 11, Art. no. 89, 2025, doi: 10.1038/s41524-025-01575-9.
[2] H. Mashhadimoslem, P. Karimi, A. Elkamel, and A. Yu, "Toward high entropy material discovery for energy applications using computational and machine learning methods," *npj Comput. Mater.*, 2025, doi: 10.1038/s41524-025-01918-6.
[3] T. Xie and J. C. Grossman, "Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties," *Phys. Rev. Lett.*, vol. 120, no. 14, Art. no. 145301, 2018.
[4] C. Chen, W. Ye, Y. Zuo, C. Zheng, and S. P. Ong, "Graph networks as a universal machine learning framework for molecules and crystals," *Chem. Mater.*, vol. 31, no. 9, pp. 3564–3572, 2019.
[5] A. Merchant, S. Batzner, S. S. Schoenholz, M. Aykol, G. Cheon, and E. D. Cubuk, "Scaling deep learning for materials discovery," *Nature*, vol. 624, pp. 80–85, 2023, doi: 10.1038/s41586-023-06735-9.
[6] X. He, Y. Chen, S. Wang, and G. Zhang, "Employing graph neural networks for predicting electrode average voltages and screening high-voltage sodium cathode materials," *ACS Appl. Mater. Interfaces*, vol. 16, no. 19, pp. 24494–24501, 2024, doi: 10.1021/acsami.4c00624.
[7] J. R. Joseph, D. H. Kiem, S. Yeom, and M. Yoon, "Interpretable graph neural networks for classifying structure and magnetism in delafossite compounds," arXiv:2512.00292, 2025.
[8] Y. Liu, C. Chen, Y. Liu, X. Zhang, and S. Xie, "Multi-objective explanations of GNN predictions," in *Proc. IEEE Int. Conf. Data Mining (ICDM)*, Auckland, New Zealand, 2021, pp. 409–418, doi: 10.1109/ICDM51629.2021.00052.
[9] J. Park, F. Sorourifar, M. R. Muthyala, A. M. Houser, M. Tuttle, J. A. Paulson, and S. Zhang, "Zero-shot discovery of high-performance, low-cost organic battery materials using machine learning," *J. Amer. Chem. Soc.*, vol. 146, no. 45, pp. 31230–31239, 2024, doi: 10.1021/jacs.4c11663.
[10] A. Jain *et al.*, "Commentary: The Materials Project: A materials genome approach to accelerating materials innovation," *APL Mater.*, vol. 1, no. 1, Art. no. 011002, 2013.
[11] R. Ying, D. Bourgeois, J. You, M. Zitnik, and J. Leskovec, "GNNExplainer: Generating explanations for graph neural networks," in *Proc. Adv. Neural Inf. Process. Syst. (NeurIPS)*, vol. 32, 2019.
[12] K. Deb, A. Pratap, S. Agarwal, and T. Meyarivan, "A fast and elitist multiobjective genetic algorithm: NSGA-II," *IEEE Trans. Evol. Comput.*, vol. 6, no. 2, pp. 182–197, Apr. 2002.
[13] Z. Li, S. Deng, Y. Liu, and J.-M. Hu, "Machine learning enabled graph analysis of particulate composites: Application to solid-state battery cathodes," *ACS Energy Lett.*, vol. 11, no. 6, pp. 4334–4342, 2026, doi: 10.1021/acsenergylett.5c04258.
[14] K. Liu, Q. Peng, Y. Liu, N. Cui, and C. Zhang, "Explainable neural network for sensitivity analysis of lithium-ion battery smart production," *IEEE/CAA J. Autom. Sinica*, vol. 11, no. 9, pp. 1944–1953, 2024, doi: 10.1109/JAS.2024.124539.
[15] X. Zhang, J. Zhou, J. Lu, and L. Shen, "Interpretable learning of voltage for electrode design of multivalent metal-ion batteries," *npj Comput. Mater.*, vol. 8, Art. no. 175, 2022, doi: 10.1038/s41524-022-00858-9.