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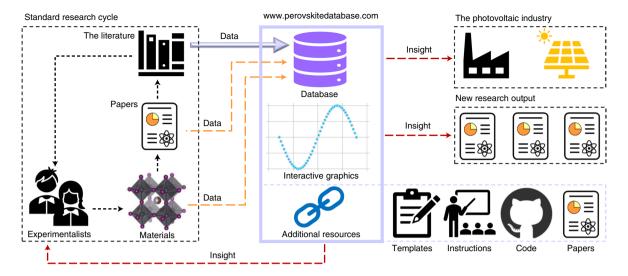
# An open-access database and analysis tool for perovskite solar cells based on the FAIR data principles

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Large datasets are now ubiquitous as technology enables higher-throughput experiments, but rarely can a research field truly benefit from the research data generated due to inconsistent formatting, undocumented storage or improper dissemination. Here we extract all the meaningful device data from peer-reviewed papers on metal-halide perovskite solar cells published so far and make them available in a database. We collect data from over 42,400 photovoltaic devices with up to 100 parameters per device. We then develop open-source and accessible procedures to analyse the data, providing examples of insights that can be gleaned from the analysis of a large dataset. The database, graphics and analysis tools are made available to the community and will continue to evolve as an open-source initiative. This approach of extensively capturing the progress of an entire field, including sorting, interactive exploration and graphical representation of the data, will be applicable to many fields in materials science, engineering and biosciences.

he halide perovskites have for the last few years been the brightest shining stars on the sky of emerging solar cell materials. They have shown great potential in optoelectronic applications such as tandem solar cells<sup>1-5</sup>, LEDs<sup>6,7</sup>, lasers<sup>8</sup>, photodetectors<sup>9,10</sup>, X-ray detectors<sup>11</sup> and for single-junction solar cells the

record certified power conversion efficiency (PCE) has reached above 25% (ref. <sup>12</sup>). The halide perovskite semiconductors thus represent a material class with considerable technological relevance where rapid development is occurring. There are, however, remaining problems related to, for example, stability<sup>13–15</sup>, scalability<sup>16–19</sup> and



**Fig. 1 | Expanding the standard research cycle in experimental material science.** An illustration of the standard research cycle and how the Perovskite Database Project can expand it by providing an open database, interactive visualization tools, protocols and a metadata ontology for reporting device data, open-source code for data analysis and so on. Solid data lines refer to data from published papers treated in this project. Dashed data lines refer to raw data from experimentation and analysed full datasets that are natural extensions to be included later. The dashed 'insight' lines represent the use of the expanded research cycle.

reliability<sup>20</sup>; the best material combinations and manufacturing processes are open questions<sup>21,22</sup>, and key standards and metrics are still under discussion<sup>23</sup>.

In the normal research cycle, researchers read papers, formulate hypotheses, generate data in the laboratory and publish new papers (Fig. 1). With historic data and insights scattered over an inaccessibly large number of papers, this process is not as efficient as it could be. At the time of writing, the keyword 'perovskite solar' does for example find over 19,000 papers in the Web of Science, making it essentially impossible to keep up to date with the literature. The perovskite field could thus be said to have a data management problem at an aggregated level.

Data have always been the foundation of empirical science, but with modern algorithms and artificial intelligence, entirely new opportunities emerge when data are collected in sufficiently large quantities and in a cohesive manner. Big data has become the lifeblood of the tech giants of Silicon Valley, the fuel for artificial intelligence and a cornerstone for the next industrial revolution<sup>24</sup>. The field of materials science is in no way oblivious to this development, and several data initiatives have been initiated, for example the Materials Project<sup>25</sup>, Aflow<sup>26</sup>, NOMAD<sup>27</sup>, the Crystallography Open Database<sup>28</sup>, the emerging photovoltaic initiative<sup>29</sup> and the inorganic crystal structure database<sup>30</sup>, to mention a few. Despite these efforts, much of the experimental materials science is still struggling to make better use of the data generated<sup>31</sup>, and notably so in applied fields where materials are often evaluated primarily by their performance in devices.

A concept of increasing importance is the FAIR data principles, that is, data should be findable, accessible, interoperable and reusable<sup>32,33</sup>. Adhering to those principles can accelerate the development and increase the return on investment as it enables cross-analysis between datasets, data reuse, as well as simplifying the use of artificial intelligence and machine learning. There is also an increased demand from government, funding agencies and journals to disseminate the underlying data accordingly. However, most laboratories are not able to adhere to the FAIR data principles, especially in the applied science fields. There are concurrent reasons behind this, including the lack of suitable data dissemination platforms. However, the largest hurdle is the diversity and complexity of

the datasets involved. For instance, sample properties are often influenced by the sample history. Furthermore, they are characterized using a large number of experimental techniques, which vary across disciplines. These small disconnected and heterogeneous datasets also require a substantial amount of metadata to be of use.

In this project, henceforth referred to as the Perovskite Database Project, we have initiated a communal bottom-up effort to transform perovskite research data management. The Perovskite Database Project aims to expand the normal research cycle by collecting all perovskite solar cell data, both past and future, in one place. Apart from making all historical data accessible and providing means to upload new experimental data, interactive graphical data visualization tools have been implemented that enable simple and interactive exploration, analysis and filtering (Fig. 1). This platform will give both academic researchers and the industry an accessible overview of what has been done before, and thereby help in finding relevant knowledge gaps and formulating new scientific questions with the hope of generating new insights, designing better experiments, avoiding known dead ends and accelerating the rate of development. The key goals of the project are to: collect all perovskite solar cell data ever published in one open-access database; develop free interactive web-based tools for simple and interactive exploration, analysis, filtering and visualization of the data; develop procedures and protocols to simplify dissemination and collection of new perovskite data according to the FAIR data principles; release an open-source code base that can be used as a blueprint for similar projects and give a few demonstrations of insights and analysis that can be easily done if all data are consistently formatted and found in one place.

# Details of the database

We have manually gone through every paper found in the Web of Science with the search phrase 'perovskite solar' up to the end of February 2020 (that is, over 15,000 papers). In total, we have manually extracted data for over 42,400 devices. While a few devices with extractable data will have slipped through our net, the devices in the database represent almost every device someone has thought is worth the effort to describe in detail in the peer-reviewed literature.

Our original data extraction protocol contained 95 attributes with metadata, process data and performance data. Those can

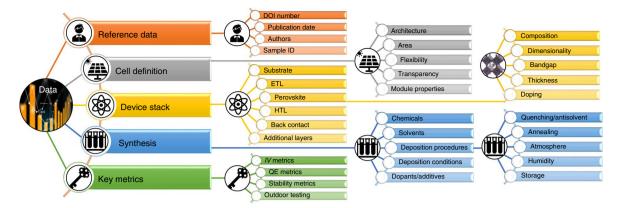


Fig. 2 | Overview of data categories in the Perovskite Database. Overview of the main categories of metadata, process data and performance data in the data extraction protocol. *IV*, current-voltage. QE, quantum efficiency.

be grouped into: reference data; cell-related data; data for every functional layer in the device stack, that is, type of substrate, electron transport layer (ETL), perovskite, hole transport layer (HTL), back contact and so on; synthesis related data for each layer and key metrics related to the performance of the resulting device; that is, current–voltage, quantum efficiency, stability and outdoor performance (Fig. 2). The categories and the formatting guidelines are described in detail in the supporting documentation. For future use, we have developed a more detailed protocol capturing up to 400 parameters per device, which can be found among the resources on the project's webpage.

Once extracted, the data have been consistently formatted according to the instruction in the supporting documentation and is now freely available in the Perovskite Database. To increase the usability of the data, we have developed interactive tools for simple exploration, analysis, filtering and visualization that can be used without programming knowledge. The code base for the project is written in Python and is available at GitHub (https://github.com/Jesperkemist/perovskitedatabase), and everyone is invited to contribute and expand the scope of the project. All the resources are found at the project website (www.perovskitedatabase.com), where they will be updated and maintained for the foreseeable future.

With all the device data consistently formatted and available in one place, a plethora of interesting possibilities opens. What follows is a small selection of analyses, visualizations and insights made possible by the Perovskite Database and the associated toolbox.

# **Example uses of the Perovskite Database**

As a first example, the perovskite solar cell development is illustrated by binning the performance for all available devices and plotting those as a function of publication date (Fig. 3a). This demonstrates the expected trend towards higher-performing devices, as well as offering a sense of the underlying variability by showing the performance distribution, and thereby providing a comprehensive view of the field's progress.

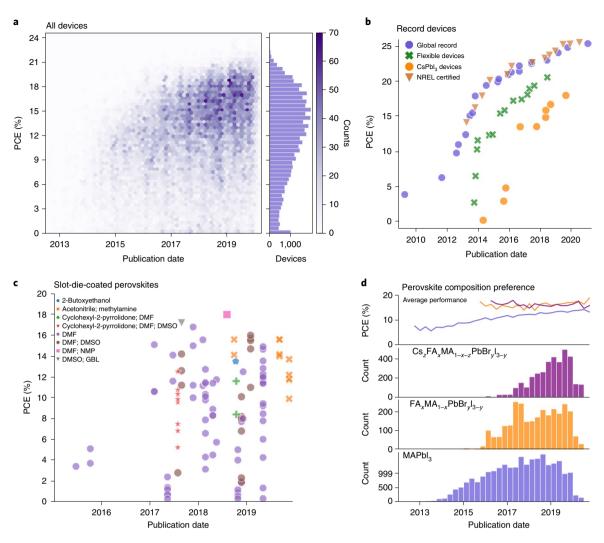
The National Renewable Energy Laboratory (NREL) efficiency chart is probably one of the most reproduced images in the photovoltaic field. It is a highly trustable source as it exclusively relies on externally certified results, but is also limited in scope. The trend in global records illustrated in the NREL chart can easily be reproduced (Fig. 3b), even if some of the data points are different as they are sorted on publication date and include non-certified data. What makes this genuinely interesting is the possibility to filter out the records for any type of cell. With a single mouse click, it is possible to display the performance evolution of, for example, flexible cells, cells based on CsPbI<sub>3</sub> or cells fulfilling any combination of constraints (Fig. 3b). With an additional click, the figure can be

downloaded and directly incorporated in presentations, applications or in a scientific publication. Clicking on a data point will also redirect the user to the original publication, which is a short-cut when searching for papers on a specific topic of interest.

A typical use case could be someone starting a project on a particular fabrication method, for example, slot-die coating. In the Perovskite Database, one simple command filters out the data for all available devices with slot-die-coated perovskites. Those data can be obtained in tabular form and downloaded with a click that gives an entry point to the key literature for further exploration. Once the relevant subset of data is obtained, it can be separated with respect to any of the dimensions represented in the database. To mention a few examples, these can be the perovskite doping conditions, the use of flexible substrates or, as shown in Fig. 3c, the solvent system used during the deposition of the perovskite. This represents a complex literature search that previously required a substantial amount of non-trivial work, but which can now be accomplished and visualized in a few minutes. With this insight at hand, it is just as easy to go on and explore additional questions, such as what is the importance of the annealing temperature, the choice of hole conductor, the antisolvent or to what extent does the perovskite composition influence the key performance metrics of the device? This illustrates a powerful short-cut towards extracting the historical data relevant for a project, for generating new hypotheses, for finding unexplored areas, for knowledge transfer and for acquiring insights otherwise easily overlooked.

With the aggregated data, it is also possible to visualize trends of how various experimental practices have been developed over the past years. An example is given in Fig. 3d that illustrates how the popularity of a few perovskite compositions, that is, MAPbI<sub>3</sub>, FA<sub>x</sub>MA<sub>1-x</sub>PbBr<sub>y</sub>I<sub>3-y</sub> and Cs<sub>z</sub>FA<sub>x</sub>MA<sub>1-x-z</sub>PbBr<sub>y</sub>I<sub>3-y</sub>, have developed over time. That figure embodies both a technical aspect of device optimization, but also the more sociological aspect of how experimental practices and ideas spread through a scientific community.

The data collected in the Perovskite Database demonstrate great flexibility to how a functional perovskite solar cell can be constructed. Among the 42,400 devices found in the database at the time of writing, there are over 5,500 unique device stacks (that is, different combinations of contact materials), not considering the more than 400 different families of perovskite compositions (that is, different combinations of the A, B and C-site ions in the perovskite ABC<sub>3</sub>-structure). More than 1,000 of these stacks have champion PCEs above 18%, and more than 300 have demonstrated PCEs above 20%. The multitude of stacks can be broken down into 1,443 unique ETL stacks, 1,957 HTL stacks, 288 back contact configurations and 194 different substrates. Some options are, however, more common than others. Around 60% of all devices are, for example,

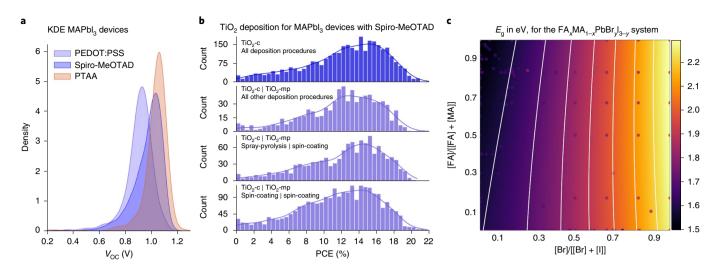


**Fig. 3 | Development of perovskite cell efficiencies.** Example of analysis from the database. **a**, Hexbin-plot of PCE measured under standard conditions as a function of the publication date for all devices in the database. Efficiency distribution for all devices is shown to the right. **b**, Evolution of record efficiency of all cells, flexible cells and CsPbl<sub>3</sub>-based cells. Data from the NREL efficiency chart are given as a comparison. **c**, Cell efficiency as a function of the publication date for slot-die-coated perovskites separated by the solvent used for perovskite deposition. DMF, dimethylformamide; DMSO, dimethylsulfoxide; GBL, gamma-butyrolactone; NMP, *N*-methyl-2-pyrrolidinone. **d**, Average performance and popularity of a MAPbl<sub>3</sub>, FA<sub>x</sub>MA<sub>1-x</sub>PbBr<sub>y</sub>I<sub>3-y</sub> and Cs<sub>x</sub>FA<sub>x</sub>MA<sub>1-x</sub>, perovskite compositions as a function of time.

based on methylammonium lead iodide (MAPbI<sub>3</sub>), and the ten most common HTLs are used in 85% of all devices, with Spiro-MeOTAD ( $C_{81}H_{68}N_4O_8$ ) used in close to half of them.

A problem faced while developing perovskite solar cells, which is in no way unique for the perovskite field, are cell-to-cell and batch-to-batch variations. Those can be large, thus masking otherwise statistically significant differences. There are also laboratory-tolaboratory variations, and what appears to make a significant difference in one laboratory may not be relevant in another. This is usually ascribed to undescribed, unexplored, unknown or hidden parameters that might influence, for example, the crystallization dynamics of the perovskite film<sup>34</sup>. Those could be things such as glove box volume, precise atmospheric composition during fabrication, minor or unintended variations in precursor stoichiometry<sup>35,36</sup>, chemical impurities<sup>37</sup> and so on to mention a few hypotheses. The Perovskite Database can mitigate that problem by combining all the available disseminated device data. That allows for more holistic conclusions about what works, what does not and how reliable and consistent various procedures are. This is illustrated with a few examples below.

In Fig. 4a, the kernel density estimation, that is, the smoothed average, of the open-circuit voltage  $(V_{oc})$  is given for three common HTLs. For a fair comparison, only MAPbI<sub>3</sub>-based devices are included. It turns out that the hole conductor has a notable impact on the  $V_{oc}$  that can be expected on average, which is an example of something that is difficult to verify with a limited number of samples produced in a single laboratory but becomes apparent with such extensive data. The figure also indicates that Spiro-MeOTAD may be associated with a small  $V_{oc}$  loss, in line with recent discussions concerning interface recombination<sup>38</sup>, and thus not be the best choice of hole conductor from a performance point of view, and the success for Spiro-MeOTAD may be more an effect of a historical coincidence, statistics and it having been heavily optimized rather than it having the highest intrinsic potential. Another example is given in Fig. 4b, which compares deposition procedures for TiO2 based ETLs in nip-devices with a MAPbI<sub>3</sub> perovskite and Spiro-MeOTAD as HTL, which are the most common ETL and HTL stacks. The very best cells have been done using spin-coated mesoporous TiO<sub>2</sub> but on an aggregated level the choice of deposition procedure has a fairly small impact and all the depicted deposition procedures



**Fig. 4 | Example of analysis from the database. a**, The kernel density estimation (KDE) of the  $V_{oc}$  for three common HTLs for MAPbl<sub>3</sub>-based devices. **b**, Performance distributions separated by deposition procedures for the TiO<sub>2</sub>-ETL in nip devices with MAPbl<sub>3</sub> and Spiro-MeOTAD. The top panel include all cells with a compact TiO<sub>2</sub> layer but without a mesoporous TiO<sub>2</sub>. The remaining panels include cells with both compact (-c) and mesoporous (-mp) TiO<sub>2</sub> layers and are separated by the deposition procedure for each layer. The solid lines are the kernel density estimates. **c**, The experimental and fitted bandgap for the FA<sub>x</sub>MA<sub>1-x</sub>PbBr<sub>y</sub>I<sub>3-y</sub> system. The background colour represents the fitted surface, the white lines are isolines and points represent the experimental data. The colour bar represents the bandgap in eV. The colour scheme gives special emphasis to outliers.

have resulted in a large spread in device performance. Excluding the mesoporous  $\mathrm{TiO}_2$  layer does not make much of a difference either for the average cell performance, which is interesting given that the very best cells still use a mesoporous  $\mathrm{TiO}_2$ -layer.

The previous examples illustrate the power of having access to large, diverse, consistently formatted and interoperable datasets. They are also only scratching the surface while raising new questions that invite further explorations by digging deeper into the data. We anticipate this dataset will be an excellent resource for future work in perovskite groups as well as in the broader machine learning and data science communities.

One of the technologically appealing aspects of the metal-halide perovskites is the tunability of the bandgap ( $E_g$ ), which ranges from below 1.2 eV for MAPb<sub>0.5</sub>Sn<sub>0.5</sub>I<sub>3</sub> (ref. <sup>39</sup>), to above 3 eV for MAPbCl<sub>3</sub> (ref. <sup>40</sup>). One way to use the collected bandgap data is to filter out perovskite compositions in a desired bandgap range. Another is to extrapolate the band gap of previously unexplored compositions, as illustrated in Fig. 4c. Here a second-degree polynomial has been fitted to the bandgap values in the database relating to composition in the FA<sub>x</sub>MA<sub>1-x</sub>PbBr<sub>y</sub>I<sub>3-y</sub> system. Conversely, in such a compositional space, a simple optical measurement could then be used to estimate the perovskite composition. With the analysis code freely available, a fitting procedure such as that in Fig. 4c could easily be done for any compositional range where sufficient data are available and it can be updated whenever new data are made available.

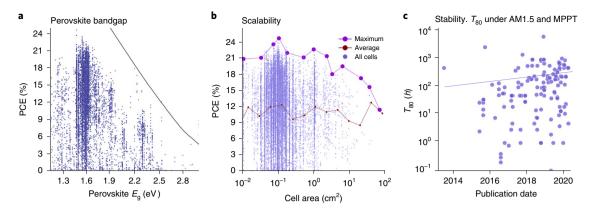
Most devices have been made with perovskites with a bandgap of around  $1.55-1.65\,\mathrm{eV}$  (Fig. 5a). That is where MAPbI<sub>3</sub> is found and it is the most interesting region for perovskite single-junction cells. For tandem integration, the need for optical matching between the subcells means that higher bandgaps are required for the top cell<sup>41</sup>. Unfortunately, from a tandem perspective, there is a drop in performance when the bandgap increases above roughly  $1.8\,\mathrm{eV}$ , with the trend continuing up to  $2.3\,\mathrm{eV}$  (Fig. 5a). This is primarily caused by an increased  $V_{\mathrm{oc}}$  loss, which probably originates from a light-induced partial phase separation in mixed Br/I-perovskites<sup>42</sup>, sometimes referred to as the Hoke effect<sup>43</sup>.

When comparing the performance as a function of the perovskite bandgap in more detail, some results are found to be unphysical as they surpass the Shockley–Queisser (SQ) limit, most frequently in terms of a too large short-circuit current. Some of those points can be explained by mislabelled or misreported bandgaps, whereas others may be caused by errors in light source calibration and aperture area. Nevertheless, this illustrates a neglect of basic error checking in historic reports.

Another major challenge towards commercial viability is scalability. Most laboratory cells have an active area  $\leq 0.2\,\mathrm{cm}^2$ , and it is also for these small cells where the highest efficiencies are found. When the cell area increases, there is a downwards trend in maximum performance (Fig. 5b), with a spike at  $1\,\mathrm{cm}^2$ , which is a common cell area used in the first step towards upscaling. The average performance is rather constant with respect to the device area. The reasons for this are unclear, but a possible explanation could be the limited number of cells larger than  $5\,\mathrm{cm}^2$  reported so far and that upscaling is primarily pursued by groups already producing high-quality small-scale devices.

Long-term stability under operational conditions is a key requirement for any photovoltaic technology, and anyone making perovskite devices, particularly with early methods and recipes, quickly realizes that this will be a challenge. There is, however, less than 20% of the cells in the database for which stability data of any kind are available. At the time of writing, the Perovskite Database contains 7,400 entries with stability data, and 5,500 of those are variations of shelf life in the dark, where devices are stored and remeasured over time. There are around 550 entries with measurements under operational conditions, that is, air mass (AM) 1.5G and maximum power point tracking (MPPT). Historical comparison of stability is complicated both by the scarcity of high-quality data and by a lack of common standards and protocols for measuring and reporting stability data. This is, however, changing due to an active discussion in the field, which recently resulted in a list of International Summit on Organic Photovoltaic Stability (ISOS) consensus protocols related to measuring and reporting of stability data<sup>23</sup>. The Perovskite Database Project is fully compatible with those ISOS protocols.

There is not one single key metric of device stability but several, all with their own merits and limitations. One of the more commonly used is the  $T_{80}$  value, which is the time it takes for a cell to lose 20% of its initial performance. In Fig. 5c, the  $T_{80}$  versus publication date is given for the nearly 120 devices in the database



**Fig. 5 | Identification of key challenges in the development of perovskite solar cells.** Remaining key challenges. **a**, PCE versus  $E_g$  for all solar cells in the database. The Shockley-Queisser limit is given as a solid line. **b**, Illustration of perovskite scalability. **c**,  $T_{80}$  versus publication date for devices measured under AM 1.5 and MPPT. The solid line represents a linear fit to data.

measured under AM 1.5 and MPPT, and where a  $T_{80}$  is stated (that is, less than 0.3% of all cells). There is a general trend towards more devices with higher stabilities as the years progress, even if we still have rather few data points. Given the importance of the problem, we expect a dramatic increase in reporting this type of data in the next few years.

Figure 5 represents a first glimpse of what is found in the Perovskite Database related to the three core technological challenges, namely tandem integration, scalability and stability. All these aspects deserve a much longer analysis, and we expect a multitude of papers to be written based on these open-source resources, both by us and by others. We intend the Perovskite Database to be a living, evolving and scalable project, and we expect future work to expand the scope of the project by adding new data, functionality, analysis, visualizations and open-source code.

# Future expansion of the database

The ambition of the Perovskite Database Project is to collect not only historic data but all future device data as well, to create a new standard for disseminating perovskite device data and to build what we can think of as the Wikipedia of perovskite solar cell research. This will require participation from the entire perovskite community, with a mental shift towards a culture where everyone feels that they can, want and will disseminate their device data by uploading it to the Perovskite Database as a complement to traditional publishing.

Uploading new data will take some time and effort. The Perovskite Database Project must therefore deliver a high degree of perceived use, simplicity, visibility, longevity and trustworthiness. In terms of use, we hope the examples in this paper, together with the interactive graphics on the project's website, have demonstrated the power of aggregated datasets adhering to the FAIR data principles, and that this alone provides an incentive to contribute. There are also other benefits to uploading one's own data. Sharing data in this way gives it new life and draws additional attention to the original publication, it is a way to comply with the demands for openness more frequently seen from taxpayers, funding agencies and publishers, and it is a service to the community that helps to accelerate the development of new solar cell technology. Finally, the tools and protocols we provide may help in organizing and improving the local data management and thereby, in the end, simplify planning, analysis and writing.

In terms of simplicity, we have developed intuitive and well-documented data extraction protocols. The backend for data cleaning and validation is written in Python, and the backend for collecting and reporting data is currently in the form of an Excel

template. The Excel template is self-explanatory, easy to use, freely available and possible to extend to fit different laboratories' internal needs. By being transparent and freely available, it is possible to build customized data pipelines that directly feed data from laboratory equipment into the template, thereby simplifying data entry even further.

Our vision is that uploading data into databases such as this one will become standard procedure as this will strengthen the associated publication by increasing its visibility and usefulness. We further anticipate involving publishers as important stakeholders in this project. Making experimental data assessible on platforms used by most of the research community will increase the visibility of scientific results. In addition, the accumulation of all device data allows an straightforward assessment as to whether reported device performance metrics are physically possible (for example, that are in the expected performance limits of the Shockley–Queisser limit for single-junction solar cells) or deviate substantially from common trends.

To ensure the project's longevity, we have secured support from the Helmholtz Organization in Germany, which acts as a guarantor ensuring that the web resources, that is, database, webpage and the GitHub account, will be operational and maintained for the coming decade, with an option of possible prolongation.

Another key aspect related to trustworthiness is the open-source nature of the project, which means transparency, to which users could suggest improvements and provide additional functionality, and it enables easy restart in case of disruption.

The database could also easily be expanded to include data relevant to, for example, LEDs, lasers, scintillators and so on, and we actively encourage initiatives in that direction.

A key problem addressed in this project is the challenge of keeping track of the field's progress when data are inconsistently formatted and scattered over an inaccessible large number of papers. A related problem is data loss, or the iceberg problem<sup>44,45</sup>. In a typical project, there may be hundreds and sometimes thousands of devices made before the paper is written. Despite this, the average number of devices for which we could extract data was fewer than six per publication with original device data. A common pattern is that one parameter is changed in few steps, and for each of those steps data for the best device could be found. Some of the data for the missing devices are presented as statistical averages, even if the data for the individual devices cannot be extracted from the papers. Data for other devices are, for various reasons, never disseminated and are essentially lost forever. Data for most of the best devices are probably disseminated, but there is a wealth of information hidden in the data now lost<sup>44,45</sup>. With the tools here developed, we facilitate

reporting data for also those kinds of device in future reports, which could mitigate the bias for not disseminating data for failed experiments and less successful devices.

#### Conclusions

In this Perovskite Database Project, we have created an open-access database for perovskite solar cell device data and visualization tools for interactive data exploration, and we have populated the database with data for over 42,000 devices described in the peer-reviewed literature up until spring 2020. We also demonstrate the capabilities of the database and the associated tools by giving a few examples of insights that can be gleaned from the analysis of this large dataset in terms of, for example, record development, tandem integration, stability and scalability. We hope that this project will prompt better data management in the perovskite field as well as a culture of data sharing, as well as inspiring other experimental fields to do the same. We could then get data with a more fine-grained data mesh and make those data available for most devices ever made, not just a few highlighted in papers as has been the case historically. In a few years, we could then have data for millions of devices, which will enable us to finally take greater advantage of machine learning and other artificial intelligence-based methods to accelerate development even further.

#### Methods

The search phrase 'perovskite solar' in the Web of Science generated over 15,000 entries by the end of February 2020. Not all of those publications relate to metal-halide perovskites and photovoltaic applications, but most do. Similarly, a few relevant papers will be missed in this search. From here, our collective team has manually gone through every paper and extracted data for all the described devices.

Of the publications we went through, we found original experimental device data in close to half of them, that is, around 7,400. Among the remaining papers, we found reviews, theoretical investigations and studies focused on material properties, as well as some non-photovoltaic-/perovskite-related publications. In total, we have manually extracted data for over 42,400 devices. The total time consumption to do this is in the range of 5,000–10,000 man hours.

On the basis of our collective experience of perovskite device development and optimization, the total number of devices ever made is probably at least two orders of magnitude larger, but for data for most of those devices cannot be extracted from the publications. In fact, data for most devices are only available as average values, in scatterplots or not disseminated at all.

One database entry per device has been the default procedure, but if only averaged data were found, we entered that as belonging to one cell but specified the number of devices the averaged is based on. Another guiding principle has been that, while preferably having all possible data for a device, having some data is better than having none. We have thus not discarded data based on poor or limited device descriptions in the scientific publications. We also considered a best estimate of a perovskite composition, for example, to be worth more than stating the information as unknown, which for example could be the case for solvent-based ion exchange procedure where the ionic fractions in the perovskite cannot be derived from the composition of the precursor solutions, but where it can be inferred from optical or X-ray diffraction data.

All data contain errors. That is unavoidable. Some sources of errors include: the data stated in the original papers are erroneous due to several possible reasons; misinterpretation of data, which is easily done when papers are ambiguous or confusingly written, and errors while transferring data from papers to the database. We have therefore set up a system for reporting dubious data points, and we thereby expect some self-correction over time, especially for data points of special interest such as records in subfields. To reduce the errors, we went through the extracted data to check for errors, misunderstandings, confusing entries and inconsistent formatting. For future data, where we expect authors to upload their own data, we expect a lower error rate than for the historical dataset. It is, nevertheless, advisable to double check outliers, especially when the applied search filters generate small datasets, so as not to draw erroneous conclusions. We also encourage authors, who know their own data best, to double check their devices in the database.

Every data point in the database is linked to the DOI number of the original publication. Every data point is thus effectively cited in the database, and for everyone who uses the data found there it is straightforward to use this DOI linkage to both find and cite the original sources of the data used.

### Data availability

The project has a dedicated website, www.perovskitedatabase.com that provide access to all resources. Among those are: the Perovskite Database, interactive

graphics exploring the database, instructions for what is found in the database, templates and instructions for uploading new data, links to all works related to the project and so on.

## **Code availability**

Codes reproducing all analyses in this paper are available in the following GitHub repository at https://github.com/Jesperkemist/perovskitedatabase.

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T.J.J. and E.U. designed the project. T.J.J. coordinated the project, wrote much of the code for the interactive graphics and wrote the first draft of the paper. M.V., A.Y.A. and O.Y. worked on coding. T.J.J., A.H., A.G.-F., A. Anand, A.A.-A., A.H., A.C., A. Abate, A.G.R., A.V., A.K., B.P.D., B.Y., B.L.C., C.A.R.P., C.R., D.R., D.F.-J., D.D.G., D.J., E.A., E.J.J.-P., E.B., E.M., G.S.A.G., G.B., G.N., G.P., G.M.-D., H.N., H.M., H.K., H.W., I.B., M.I.D., I.B.P., I.E.G., J.N.V., J.D., J.K., J.Y., J.L., J.A.S., J.P., J.J.J.-R., J.F.M., J.-P.C-B., J.Q., J.W., K.S., K.H., K.D., K.F., L.M., L.A.C., M.H.A., M.V.-M., M.A.R.-P., M.A.F., M.V.K., M.G., M.K., M.S., M.A., N.A., O.S., O.M., O.S.G., P.F., Q.Z., R.B., R.M., R.P., S.S., S.A., S.K., T.U., T.A., T.E., T.W.D., U.W.P., W.Z., W.F., W.Z., V.R.F.S., W.T., X.Z., Y.-H.C., Z.I., Z.X. and E.U. all contributed to the laborious task of going through the literature, extracting the data found there and formatting consistently. All authors have participated in preparing the final draft of the paper.

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#### Competing interests

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