SPRINGER NATURE COLLABORATES WITH DUKE UNIVERSITY ON PEROVSKITE DATA

Duke University has been licensing SpringerMaterials since 2013. In 2022, Duke University’s Associate Professor in the Department of Mechanical Engineering and Materials Science, Prof. Volker Blum, started a collaboration with Springer Nature as a result of his perovskite research. To ensure longevity of the data and reach a wider audience Prof. Blum started working with the SpringerMaterials team on adding his perovskite research data to the SpringerMaterials platform.
During this collaboration, Prof. Volker Blum and his research group assembled and curated a materials database focused on perovskite semiconductor materials, in collaboration with SpringerMaterials and in the spirit of the Landolt-Börnstein collection. The proposed collection focused on providing the “best available” data for a given material and/or property, irrespective of whether the data originates from experiment or theory. Additionally, new data was systematically added by computational predictions of materials properties where such an approach was possible with high fidelity.

The approach was divided into two steps:

1. Digitising key materials data for inorganic perovskites from the traditional Landolt-Börnstein collection: The team aimed to provide roughly 4000 datasheets (2000 each year) in SMI 3.0 format and worked with the SpringerMaterials team on any changes necessary to make these datasheets ingestible into the platform.

2. Providing necessary support to incorporate and further refine materials data collected in the open, NSF-funded “HybriD3” database for hybrid organic-inorganic perovskites, which Prof. Blum’s group has been continuously developing. (Springer Materials is an unfunded collaborator in the NSF-DMREF project.) This data collection now covers about 400 compounds and will continue to be enhanced. Newly added data will be carried over to SpringerMaterials as well.

The project started in 2022 and over the following two years, Ryan Chakraborty, a post-doctoral researcher from Duke University is working on the digitisation and further support to incorporate data into the platform. The curation of existing inorganic perovskite materials data and the carry-over of organic-inorganic hybrid materials data is occurring simultaneously throughout the project.
The importance of perovskite materials in renewable energy

The global perovskite market size is projected to grow from $84 million in 2021 to $1.1 billion by 2026, at a compound annual growth rate of 66.5%. The increasing demand for renewable energy sources and the development of next-generation solar cells are driving the growth of the perovskite market.¹

In the early 2010s, solar cell technology saw the emergence of a new class of solar cells based on mixed organic-inorganic halide perovskites.² The benefits of halide perovskites are their high performance and low production costs in solar cells. According to National Renewable Energy Laboratory (NREL) perovskite solar cells have shown an increase in efficiency from about 3% in 2009 to over 25% in 2023. However, according to latest research there are still some challenges that must be overcome for perovskite technologies to become commercially successful. Institutions such as Solar Energy Technologies Office (SETO) and the European Commission³ are supporting research around Perovskite through specific funding programmes.

On 13th August 2020, the U.S. Department of Energy announced a funding program to support research and development advancing perovskite photovoltaic devices and selected 22 projects to receive $40 million on 25th of March 2021. The research projects will focus on improving the understanding of perovskite stability to enable domestic production of high-efficiency perovskite devices. In addition, a center to develop test protocols that enables confidence in the long-duration field performance of perovskite-based PV technologies will be established for researchers, bankability experts, and performance engineers.⁴

¹Perovskite Solar Cell Market, Markets and Markets
²The emergence of perovskite solar cells, Nature Photonics
³Stable high-performance Perovskite Photovoltaics, European Commission
⁴Solar Energy Technologies Office Fiscal Year 2020 Perovskite Funding Program, U.S. Department of Energy
### Perovskite research funding from the last 5 years (Sources: SN Insights)

<table>
<thead>
<tr>
<th>Funders</th>
<th>Aggregated funding amount for each item</th>
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<tr>
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Source: https://insights.dimensions.ai

Criteria: ‘perovskite solar cells’ in full data, start year is 2018 or 2019 or 2020 or 2021 or 2022 or 2023.

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What are perovskite materials?

A perovskite is any material with a crystal structure similar to the mineral called perovskite, which consists of calcium titanium oxide (CaTiO3).

The most prominent application of perovskite is in solar cells. Perovskite solar cells have achieved high efficiency levels, reaching up to 25.5% in the lab. They can be fabricated using low-cost materials and simple manufacturing processes, making them an attractive alternative to traditional silicon solar cells.

Traditional inorganic perovskite materials as well as the related hybrid organic-inorganic perovskites, form a vast space of functional materials. Traditional functional materials applications of perovskite materials span, e.g., ferro- and piezoelectricity, catalytic applications, and high-temperature superconductivity. Hybrid organic-inorganic perovskites add a broad range of new semiconductor applications, spearheaded by low-cost depositable solar cell absorber materials that have led to remarkable device efficiencies in a span of only about a decade. This success has spawned a very large community of researchers in academia and industry that is now focused on discovering and developing new crystalline hybrid-organic semiconductors based on the perovskite paradigm. As one example, a recent review by Saparov and Mitzi, Chem. Rev. 116, 4558-4596, has been cited almost 1,000 times since it first appeared in 2016.

Especially the new materials developments in the organic-inorganic perovskite space have led to a vast, rapidly increasing universe of materials data that is now being collected largely in a bottom-up fashion. This includes both high- and low-quality data, leading to some significant scatter even for seemingly simple materials properties (e.g., phase transition temperatures) across different sample types, quality, synthesis procedure, etc. The materials in question can contain complex organic functionalities, leading to versatile opportunities for materials optimization, but at the same time rendering simple high-throughput data collection techniques ineffective. Overall, there is therefore a strong need for a careful, curated, trusted perovskite materials data collection in the community.
Duke University's has been using SpringerMaterials since 2013

Long before the collaboration, Prof. Blum was using Duke University's SpringerMaterials licence for his research, relying heavily on the Landolt-Börnstein series when starting his career as a physicist. The first collaboration between Prof. Blum and SpringerMaterials involved digitising content from the semiconductor volumes of the Landolt-Börnstein series, making the data machine-readable, so it could be ingested into SpringerMaterials interactive platform.

The Landolt-Börnstein series

The Landolt-Börnstein (LB) book series has been published by Springer since the year 1883. It is the heart of SpringerMaterials, the world's largest database of curated data on materials and their properties. The objective of the sponsored research project is to convert text, figures and typeset tables from pdf versions of 15 LB volumes dedicated to semiconductors into machine readable formats that allows users to access them using interactive tools/features.

About Duke University

Duke University is a private research university in Durham, North Carolina, United States. The institution was founded in the present-day city of Trinity in 1838 and moved to Durham in 1892. The campus consists of three contiguous sub-campuses in Durham and a marine lab in Beaufort spanning over 8,600 acres in total.

Duke University is one of the ten largest research universities in the United States spending more than $1 billion on research per year. As of 2019, amongst its alumni's are 15 Nobel laureates and 3 Turing Award winners, as well as 50 Rhodes Scholars.

About SpringerMaterials

SpringerMaterials provides curated data and advanced functionalities to support research in materials science, physics, chemistry, engineering, and other related fields. The database is a comprehensive resource of curated data covering 3,000 properties and over 300,000 materials on one platform:

The SpringerMaterials platform offers:

- Enhanced data visualization features display interactive crystal structures, data tables, and phase diagrams with export options for further analysis
- Search functions optimized for materials science like elemental composition or chemical structure searching to quickly find material property data
- Trusted and curated resource with thousands of materials science experts ensuring high data quality

“Materials Science today is a data-driven science. Scientists are able to calculate most of the physical properties of a material using computational methods. However, experimental data is needed for benchmarking and validating calculated values. That’s where the Landolt-Börnstein books come into the picture, because they contain large collections of carefully curated experimental data. However, this data is buried within books and cannot be easily accessed and exported into software tools. Converting these books into machine-readable data sets allows scientists to incorporate this data easily into their workflows.”

– Prof. Volker Blum, Duke University

Find out about SpringerMaterials and request a trial