Science and Technology Facilities Council

Hartree Centre

Transforming solar cell materials discovery with AI prediction

STFC Hartree® Centre worked with Swansea University through the Hartree National Centre for Digital Innovation (HNCDI) programme to develop an AI pipeline that could accelerate next-generation solar cell discovery.

Challenge

Solar cells convert sunlight into electricity by generating and transporting electrical charges within their materials. To enable wider adoption of solar power, new solar cells must achieve higher efficiencies, lower production costs, and improved sustainability. High-efficiency organic solar cells employ an active layer composed of two materials: a donor and an acceptor, both of which can absorb light, generate charges, and therefore contribute to the generation of electrical current. Device performance is characterised by key photovoltaic parameters such as the short-circuit current density, open-circuit voltage, and fill factor, which together determine the power conversion efficiency (PCE). Small changes in molecular structure can strongly influence these parameters and, consequently, the overall PCE. Traditionally, the discovery of improved donor–acceptor materials for high-performance organic solar cells has relied on slow and expensive experimental trial-and-error approaches, due to the lack of reliable, efficient screening methods.

Approach

The HNCDI team developed the Helios framework which combines molecular structure data with solar cell device measurements and uses deep learning to predict PCE. This enables computational screening to run in-silico experiments, identify the best candidates based on PCE early, and narrow the list to a small set of promising materials for experimental validation. The Helios pipeline standardises data cleaning, feature generation, training, and inference into a reproducible workflow with a command line interface and documented demos. Helios reports standard accuracy and error metrics, showing the trained model captures most of how PCE changes and keeps prediction errors low enough for practical screening. Consistent data splits and scaling keep the evaluation reliable and repeatable.

> **“Helios offers the opportunity to direct the design of new organic photovoltaic materials, accelerating material choices in the drive to improve device efficiency and lifetime.”**

Peter Holliman
Swansea University

Credit: Adobe Stock

Benefits

Helios enables rapid screening of candidate materials, dramatically reducing the number of experiments needed to identify high performing molecules combinations. This shortens R&D cycles, reduces waste, and supports sustainable innovation in photovoltaic materials. With an available, documented pipeline and example notebooks, researchers can integrate Helios into their workflows and explore a wider materials discovery space faster than traditional trial and error methods. Helios is also well-positioned to expand beyond PCE to predict other outcomes such as device lifetime, and to be retrained on larger datasets to boost accuracy and coverage.

At a glance

- Framework identifies best candidates for power conversion efficiency
- Helios standardises data cleaning, feature generation, training, and inference into a reproducible workflow
- Dramatically reducing the number of experiments needed to identify high performing molecule combinations
- Shortens R&D cycles, reduces waste and supports sustainable innovation

The programme

The Hartree National Centre for Digital Innovation is a collaboration between the Hartree Centre and IBM which offers a safe and supportive environment for UK organisations to explore the latest digital technologies and skills, develop proofs-of-concept and apply them to industry and public sector challenges.

Who we are

The Hartree Centre was created by UK Government to help businesses and public sector organisations accelerate the adoption of high performance computing (HPC), big data analytics, artificial intelligence (AI) and quantum technologies. We play a key role in realising UK Government's Industrial Strategy by stimulating applied digital research and innovation, creating value for the organisations we work with and generating economic and societal impact for the UK. We are proud to be part of UK Research and Innovation.

What we do

- Boost productivity and innovation for industry
- Offer training and skills development
- Provide insights into future technologies
- Give tailored business development support