Computational photovoltaics

Can machine learning predict power conversion efficiency of organic photovoltaics?
ABSTRACT: In this paper, the ability of three selected machine learning neural and baseline models in predicting the power conversion efficiency (PCE) of organic photovoltaics (OPVs) using molecular structure information as an input is assessed.

Can machine learning predict the PCE of organic photovoltaics based on molecular structure information?
In this paper, the ability of five machine learning models and HDMR to predict the PCE of organic photovoltaics based on molecular structure information is assessed, including the impact and implications of the choice of training data.

Are organic photovoltaic materials a good candidate for Cheap solar cells?
Provided by the Springer Nature SharedIt content-sharing initiative Organic photovoltaic (OPV) materials are promising candidatesfor cheap,printable solar cells. However,there are a very large number of potential donors and acceptors,making selection of the best materials difficult.

Why should you use our framework for organic photovoltaic chemistry?
Our framework evaluates the chemical structure of the organic photovoltaic molecules directly and accurately. Since it does not involve density functional theory calculations,it makes fast predictions. The reliability of our framework is verified with data from previous reports and our newly synthesized organic molecules.

Which molecule is used for photovoltaic performance?
We further investigated the photovoltaic performance of these functional molecules using the conventional device structure described in the experimental part. In addition, we adopted both conventional fullerene acceptor PC 71 BM as well as recently emerged non-fullerene molecule Y6 as the electron acceptor.

It is a time-consuming and costly process to develop affordable and high-performance organic photovoltaic materials. Computational methods are essential for accelerating the material discovery ...

Abstract This study analyses the fluid dynamics of wind loadings on the floating photovoltaic (PV) system using computational fluid dynamics. The two representative models of pontoon-type and a frame-type with a panel angle of 15 to the ground were investigated. The simulation was performed using the steady solver

Photovoltaic Modeling Handbook Scrivener Publishing 100 Cummings Center, Suite 541J Beverly, MA 01915-6106 Publishers at Scrivener Martin Scrivener (martin@scrivenerpublishing) Phillip Carmical (pcarmical@scrivenerpublishing) Photovoltaic Modeling Handbook Edited by Monika Freunek Müller

The viscoelastic response of backsheet materials significantly affects the durability of the photovoltaic (PV) module. In this study, the viscoelastic response of commercially available backsheet materials is

experimentally characterized and computationally modeled. An extensive viscoelastic experimental study on backsheet materials is carried out, considering the ...

Mg 2 CrN 3, Mg 2 MnN 3, MgVN 2, ZnVN 2 and X 2 BiN 3 (X = Mg, Ca, and Sr) are expected to achieve ferroelectric photovoltaics property with a strong visible light harvest and high carrier mobilities. The low 3 d transition metals or Bi elements in ternary metal nitrides could play an important role in achieving high ferroelectric photovoltaics ...

MIT researchers have developed a computational simulator that can help predict whether changes to materials or design will improve performance in new photovoltaic cells. ... A new system both predicts the efficiency of new photovoltaic solar cell materials and shows how much different input parameters affect output. Credits: Image: MIT News ...

Classic ferroelectric photovoltaic materials BiFeO 3 displays an anomalously large photovoltage attributed to the domain wall effect [5]. In our computational study of ferroelectric ternary nitrides, we operated under the assumption that these materials behaved as single-domain ferroelectric compounds, overlooking the influence of domain walls.

In light of these consid-erations, the aim of this paper is to critically test the ability of machine learning models to predict the PCE of organic photovoltaics based on the SMILES-derived ...

Organic photovoltaic (OPV) materials are of great interest because of their potential to generate cheap, printable semiconductor devices that convert light into electrical energy. ...

Reviewing the related literature shows that radiation tracking is the most applied method for optical modeling of photovoltaic panels . To this aim, a photovoltaic panel is assumed as a set of layers with different optical properties. These layers have long lengths and widths relative to their thicknesses.

Internet of things (IoT) has necessitated the development of indoor photovoltaics to enable a web of self-powered wireless sensors/nodes. We analysed a CsPbI3 wide band gap perovskite for indoor photovoltaic application. An Indoor photovoltaic (IPV) device based on CsPbI3 showed a theoretical efficiency of 51.5% at a band gap of 1.8 eV under indoor light ...

npj Computational Materials - Machine learning-enabled chemical space exploration of all-inorganic perovskites for photovoltaics ... Because MHPs with indirect bandgaps are not usually suitable ...

Organic photovoltaic (OPV) cells provide a direct and economical way to transform solar energy into electricity. Recently, OPV research has undergone a rapid growth, and the power conversion efficiency (PCE) has ...

Computational modeling, Machine learning, Molecular structure, Abstract. In this paper, the ability of three

selected machine learning neural and baseline models in predicting the power conversion efficiency (PCE) of organic photovoltaics ...

Organic Photovoltaic Solar Cells. NREL has strong complementary research capabilities in organic photovoltaic (OPV) cells, transparent conducting oxides, combinatorial methods, molecular simulation methods, and atmospheric processing. ... We have the scientists and the tools to combine molecular design using computational resources with organic ...

This Perspective introduces the Harvard Clean Energy Project (CEP), a theory-driven search for the next generation of organic solar cell materials, and gives a broad overview of its setup and infrastructure, present first results, and outline upcoming developments. This Perspective introduces the Harvard Clean Energy Project (CEP), a theory-driven search for ...

Photovoltaic (PV) systems are increasingly becoming a vital source of renewable energy due to their clean and sustainable nature. However, the power output of PV systems is highly dependent on environmental factors such as solar irradiance, temperature, shading, and aging. To optimize the energy harvest from PV modules, Maximum Power Point Tracking ...

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This article presents a comprehensive 3D mathematical model and numerical simulation for solar photovoltaic thermal (PV/T) systems that will be helpful for optimizing the system performance. The simulation has been done in COMSOL Multiphysics® software.

Shift current photovoltaic devices are potential candidates for future cheap, sustainable, and efficient electricity generation. In the present work, we calculate the solar-generated shift current ...

The proposed heat sink was designed as an aluminum plate with perforated fins that is attached to the back of the PV panel. A comprehensive computational fluid dynamics (CFD) simulation was ...

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the organic photovoltaic and the underlying properties of the materials, as they can make use of existing computational and experimental data and make predictions at a fraction of the cost. A wide variety of machine

learning algorithms have been applied to predict the performance of organic photovoltaics using different target datasets.

computational chemistry; organic photovoltaics; Disclosure statement. No potential conflict of interest was reported by the author(s). Additional information Funding. This research was supported by the Agencia Nacional de Investigación y Desarrollo (ANID) through FONDECYT 11181205 and UTA-Mayor 4757-21 research grants. Powered@NLHPC: Work ...

The physics of photon absorption, exciton and free carrier generation, relaxation, transport, recombination, and collection is analyzed and compared, step-by-step, between photosynthetic complexes and photovoltaic cells. By unifying the physics of the biological photosynthesis process and the device physics of photovoltaic cells, it is shown that well ...

The attributes and limitations of DFT for the computational design of materials for lithium-ion batteries, hydrogen production and storage materials, superconductors, photovoltaics and ...

Abstract This study analyses the fluid dynamics of wind loadings on the floating photovoltaic (PV) system using computational fluid dynamics. The two representative models of pontoon-type and a frame-type with a panel angle of 15° to the ground were investigated. The simulation was performed using the steady solver and incompressible Reynolds-Averaged ...

Abstract Over past two decades, organic photovoltaics (OPVs) ... [54, 55] Hence, a very high computational cost is still required when high-throughput screening is utilized for molecule design. ML could accelerate this progress to a large extent. As is listed in Table 1, ...

Computational modeling sheds light how grain-boundary charge can affect solar cell current collection. Also available is NREL"s Photovoltaic (PV) Optics software package that was specifically developed for designing solar cells and modules ...

The viscoelastic response of backsheet materials significantly affects the durability of the photovoltaic (PV) module. In this study, the viscoelastic response of commercially available backsheet ...

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