Optimizing Materials Discovery for Photovoltaics (PV) in Space
Entangled Energy

Soheil Mirzarasouli, Mohammed Alahmady Abdullah,
Puja Chakraborty, Maria Nicos Alain Pasaylo

Contents

1 a.) Problem Statement and Background

More renewable energy resources are being incorporated into power grids [8]. One promising resource is photovoltaic (PV) cells, which convert sunlight into electricity. PV cells are not only crucial for application on Earth, but also aerospace applications, such as satellites, space stations, and powerplants [9–11]. They provide a reliable energy source in space environments and are now being considered for data centers in space [12, 13]. However, the materials currently used for PV cells on Earth, such as single-junction devices based on Si, are not best suited for space missions [14]. There are many factors to consider in the space environment, such as the spectrum of sunlight outside Earth's atmosphere, extreme temperature fluctuations, and high radiation levels, all of which affect PV efficiency [8].

Considering these applications and conditions, our team thinks it is important to find ways to discover new materials that can adapt to the space environment and optimize energy production. Furthermore, this is interesting because of the current quantum and AI applications in aiding with discovering these new materials. Our team mainly focuses on answering the following question: How to accelerate finding the best candidate materials in reducing the degradation effects of solar radiation on solar cells?

2 b.) Background Research and Literature Review

Photovltaics, PV, for use in space typically consist of a substrate, cement, cover glass, and solar cells [15]. These PVs have many applications in the space environment. One example are the PVs used for the International Space Station (ISS) which can generate 110kW of power that can supply 46kW of continuous power for research experiments after battery charging, life support, and distribution [16].

2.1 Space Conditions

There are several factors to consider when using PV in the space environment. The Air Mass Zero (AMO) spectrum is the spectrum outside of Earth's atmosphere and typically decreases overall cell efficiency [16]. Another factor is temperatures as it is directly related to operating temperature, and thermal cycles can cause cracking of components and delamination of several layers [14, 16, 17]. At 300 km, 80% of the atmosphere is highly reactive atomic oxygen which erodes polymers and composites that might in array substrate and silver interconnects between solar cells [14, 16]. Solar winds can induce surface charging, electrostatic discharge, power loss, and short circuit in the electronic and PV components [14]. There are also naturally occurring meteoroids and man-made space debris, but damage to PVs in the past were mainly from erosion and cracking of cover glass [14, 16].

For our project, we focus on the solar cell degradation due to solar radiation. Solar radiation can damage PVs through ionization and formation of defects, and its main effect is on the open-circuit voltage, the short circuit current, and maximum power of the cell [14, 17]. Radiation degradation in space solar cells is influenced by factors such as particle type, energy and fluence, shielding, and cell design [16]. We decided

to focus on solar radiation because it is the most dangerous for stability and lifetime of the solar cells [14].

There have been attempts to simulate the space solar environment, but this has been difficult. JPL has been able to determine the solar radiation damage in solar cells made up of silicon and gallium arsenide [16]. The JPL-91 model, developed by the Jet Propulsion Laboratory, is highly accurate but relies on extensive empirical measurements [18].

NRL created a model for the displacement damage dose based on the non-ionizing energy loss [16]. There are also models for mapping particle fluxes and interplanetary proton fluence [17]. Additionally, NASA developed the Solar Array Verification and Analysis Tool (SAVANT) for solar cell analysis, and it was able successfully to predict the degradation of GaAs/GE and $CuInSe_2$ [16].

The NIEL approach, researched by the U.S. Naval Research Laboratory, correlates damage from various energies of protons and electrons based on the rate of energy transfer to the cell lattice [19]. The displacement threshold energy is used to determine the defect formed by irradiation of high-energy particles [20]. For our project, we input displacement threshold energy to the calculator for the Screened Relativistic (SR) Non-Ionizing Energy Loss (NIEL) curve for a particle incident on a material and OMERE for the solar cell degradation simulator [21, 22].

One crucial aspect of space-related materials is their end-of-life (EOL) performance that OMERE is able to calculate. For PV cells, EOL pertains to their performance after prolonged exposure to the space radiation environment, primarily consisting of protons and electrons trapped in Earth's magnetic field, as well as solar protons [17].

2.2 Materials for Photovoltaics in Space

To address some of these differences in the space setting, there are different constructions for PV in space compared to PVs used on Earth [23]. There are PVs that also include an aluminum honeycomb core with carbon fiber face sheets so that they can survive the mechanical loads during launch and maintain a constant sun-facing position in orbit [17]. The cover glass acts as a shielding that reduces radiation damage to the solar cell by reducing the low-energy peak in the proton spectrum [17]. The surface area of the array is also an important factor. The larger the array and the further it extends from the satellite, the larger the disturbing torques are on the satellite [17]. Electroluminescence Imaging can be used to detect mechanical defects when the solar cells have cracks which might propagate during a thermal cycle [17].

For our project, we will focus on the materials for PV cells. To measure how well a PV is performing, there is a metric called power conversion efficiency (PCE). Power conversion efficiency is the amount of electrical energy the PV can produce compared to the energy from the light energy it is receiving, and one of the important properties that determines the PCE of the solar cell is the bandgap [23]. The fundamental aspects for optimizing SCs are light absorption and generation of carriers, separation and transport of charge carriers, and collection of charge carriers [14]. Here we explore some current materials and alternative candidates used for solar cells in space (Note that this table is in progress and we plan to compile more information here).

2.3 Methods for Materials Discovery

There have been many solutions to discovering new materials. Here we will explore some methods in materials discovery and discuss their advantages and disadvantages.

2.3.1 DFT [1, 2]

The Density Functional Theory (DFT) is based on the idea that the ground state properties of a many-electron system can be determined using functionals of the electron density, rather than the many-body wave function. This simplifies the calculations significantly.

Advantages

- Predictive power: Accurately predicts properties of materials before they are synthesized.
- Cost-effectiveness: Computational screening is much cheaper and faster than experimental testing.
- Access to atomic-scale information: Provides insights into electronic structure and bonding that are difficult to obtain experimentally.

Disadvantages

- Accuracy: The exact exchange-correlation functional is unknown, leading to approximations that can affect accuracy.
- Computational cost: For large systems or highly correlated materials, DFT calculations can be computationally expensive.
- Excited states: Standard DFT is a ground state theory and may not accurately describe excited state properties.

2.3.2 VQE [3, 4]

Quantum Variational Eigensolvers (VQEs) are hybrid quantum-classical algorithms designed to find the ground state energy and wavefunction of quantum systems. They are particularly useful for problems in quantum chemistry and materials science.

Advantages

- Hybrid Nature: Leverages both quantum and classical resources efficiently.
- Noise Resilience: Generally more robust to quantum hardware noise than purely quantum algorithms.
- Flexibility: Can be adapted to various problem types and hardware constraints.

Disadvantages

- Scalability: UCCSD ansatz generates deep quantum circuits with a large number of parameters to be optimized, limiting its applicability on noisy near-term quantum devices only to the simplest chemical systems.
- Ansatz Expressibility: The chosen ansatz may not be able to represent the true ground state.

2.3.3 DFT+VQE [5]

Combining Density Functional Theory (DFT) and Quantum Variational Eigensolvers (VQEs). DFT is used for high-throughput screening of candidate materials Identify promising structures and compositions. VQE is used to refine properties of selected candidates focus on properties where DFT may be less accurate. They specifically use ADAPT VQE that relies on wave function ansatz that grows iteratively unlike VQE where its accuracy and efficiency depends on parametrized ansatz of the wave function.

Advantages

- Improved Accuracy: Overcome limitations of each method alone.
- Computational Efficiency: Use DFT where it's sufficient, VQE where higher accuracy is needed.
- Broader Applicability: Address a wider range of materials and properties.
- Validation: Cross-validate results between methods.

Disadvantages

- Method Compatibility: Ensure consistent basis sets and approximations between DFT and VQE.
- Scale Mismatch: Bridging the gap between large-scale DFT and smaller-scale VQE calculations.
- Resource Allocation: Determining when to use each method for optimal efficiency.
- Interpretation of Results: Developing frameworks to combine and interpret results from both methods.

2.3.4 DFT+eDMFT [6]

Density Functional Theory (DFT) combined with dynamical mean field theory (DMFT). First, the electronic potential calculated. Then, they solve eigenvalue problem for Kohn-Sham orbitals and adds spin-orbit coupling. The local green's function and hybridization function are calculated, and the auxiliary impurity problem for electronic self-energy correction is solved for. Lastly, they calculate the DMFT+DFT valence electronic charge by adding core states to DFT charge and mixing electronic charge density

Advantages

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2.3.5 ML+DFT [7]

Combined with Machine Learning (ML) combined with Density Functional Theory (DFT). The Spectroscopic Limited Maximum Efficiency (SLME) for non metallic materials is calculated. They trained a supervised machine learning classification model to predict the high-efficiency SLME with a threshold of 10% using classical force-field inspired descriptors (CFID) and gradient boosting decision trees (GBDT) algorithm. They calculated DFT using Vienna ab initio simulation package (VASP).

Advantages

- Faster Prediction: Quickly identify whether a material has SLME above 10%.
- Reduced Quantum Computation: Screening process allows for less DFT calculation cost.

Disadvantages

- Computational Cost: Enormous calculation for G_0W_0, one of the methods used to calculate the SLME, with and without spin-orbit coupling.

3 c.) Our Application of AI and Quantum Methods

3.1 Our Proposed Approach

For our approach, we use supervised machine learning to narrow down the search space of candidate materials to run the quantum method, for DFT in eDMFT, less since it requires more computation hardware. Figure 1, summarizes the steps of our process described below:

1. Training and testing a binary classifier to identify suitable and unsuitable candidates (See our demo code for more details).
   (a) Our data comes from JARVIS, and it includes different materials along with descriptions like band gap, exfoliation energy, dimensionality [24].
   (b) To create a dataset, we take the values which have existing SLME values. These values estimate the theoretical PCEs of PVs [25]
   (c) For our case, we follow criteria where we mark a material suitable if SLME value >= 10% [7]. Our data set consists of 9770 materials. We add the additional column with 1 for when a material SLME value>= 10%. Otherwise, we mark it with 0.
   (d) We remove any columns related to SLME values from this dataset, and we split our dataset into 80% training and 20% testing. Our training set consists of 7,816 materials and our test set contains 1,954 materials.

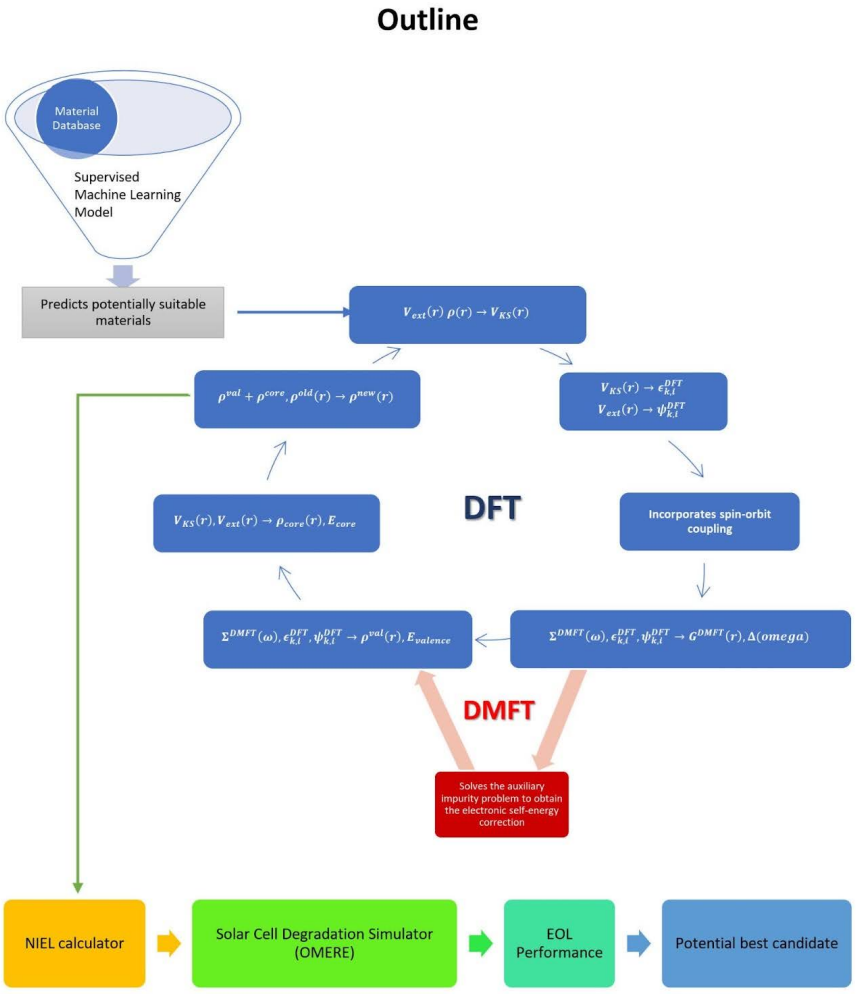


Fig. 1 Outline of our pipeline for materials discovery for PV in space.

(e) For preprocessing our data, we drop some of the columns so that we are left with categorical and numerical values. We then convert them to the appropriate data type (i.e. integers, floats, and booleans). These will be the features that our model will use to predict outcomes.

(f) We set the model hyperparameters based on this paper's findings [7]. We use the Light Gradient Boosting Machine (LightGBM) as our method [26]. LightGBM is based on decision trees that improves the model's efficiency and reduce memory

storage, and we decided to use it because of its speed, higher accuracy, and capabilities to handle large data compared to other boosting algorithms [27].

(g) After training the model, we then make predictions with our model using our test set.

(h) For evaluation of our model's performance, we use a confusion matrix, classification report, and the area under the Receiver operating characteristic curve (ROC AUC).

(i) For our confusion matrix in Figure 2, our model was able to predict a large number of true negatives (top left quadrant) and true positives (bottom-right quadrant). This means that it is performing well in identifying which materials are potentially suitable or not from the 1,954 materials in our testing set.

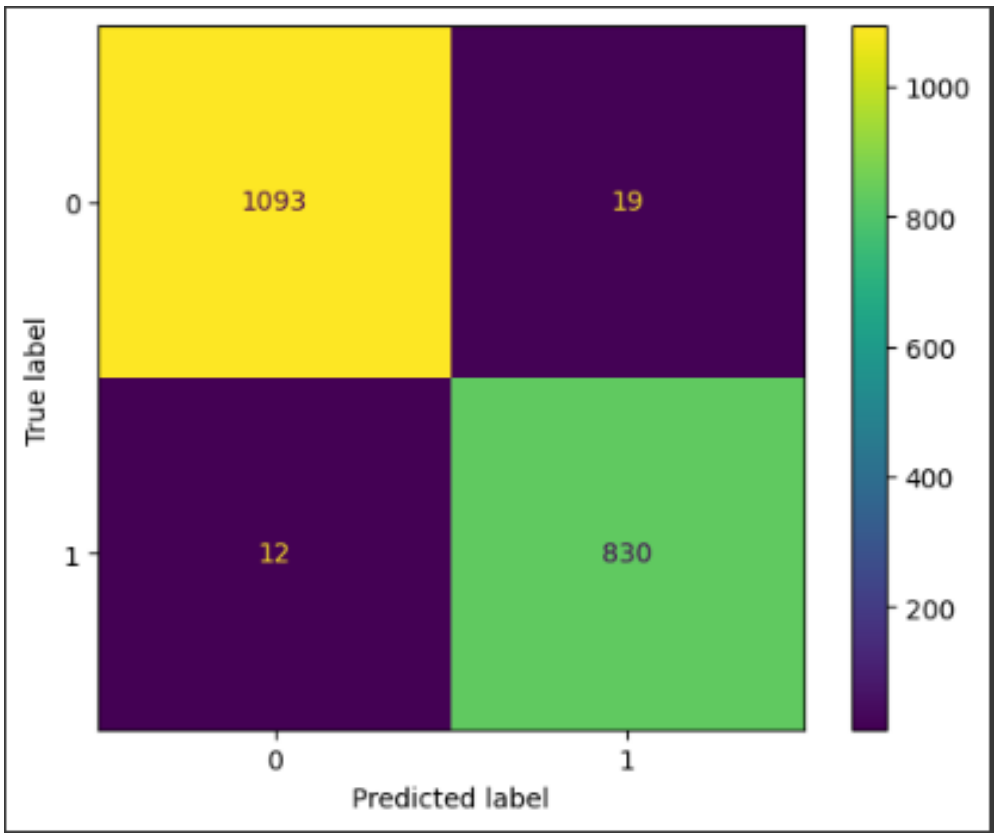
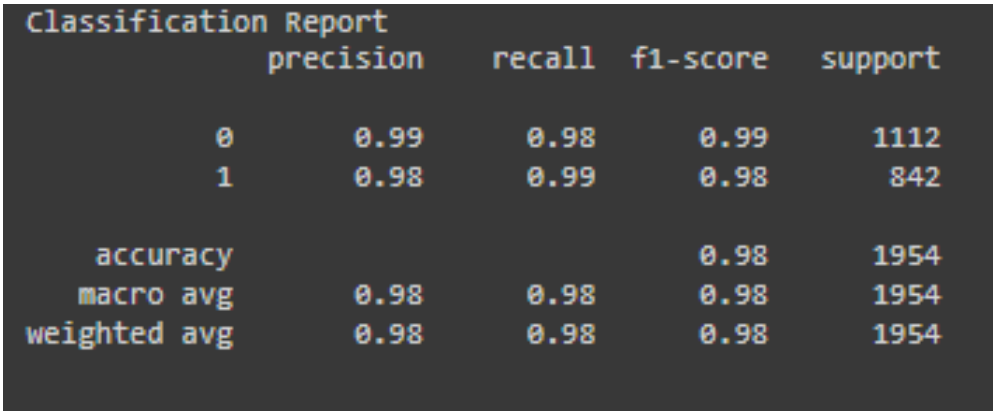


Fig. 2 Confusion Matrix results for test set with 1954 materials

(ii) For the classification report in Figure 3 , we have an accuracy of 98%. This is the proportion of predictions that the model predicted correctly.



Classification Report

	precision	recall	f1-score	support
0	0.99	0.98	0.99	1112
1	0.98	0.99	0.98	842
accuracy			0.98	1954
macro avg	0.98	0.98	0.98	1954
weighted avg	0.98	0.98	0.98	1954

Fig. 3 Classification report for test set with 1954 materials

(iii) The ROC AUC is the aggregate measure of performance across all possible classification thresholds. The ROC AUC for our model is 0.98. The curve plots the possible true positive rates against false positive rates so a value closer to 1 indicates that our model performs well.

2. We then pass the structure of the materials that we find suitable from our previous step. We employ the DFT+eDMFT approach to calculate the threshold displacement energy (E_d) [28, 29].
   (a) We conduct the phonon calculation using the "frozen phonon" approximation, also known as the "Finite Displacement Method". In this approximation, after obtaining the material structure, we use the Phonopy package [30, 31] to generate structures with atoms displaced according to the symmetry of the system.
   (b) Next we should run eDMFT. We can repeat the DMFT loop for self-energy computed by the impurity solver, and DFT loop for electronic charge, multiple times to achieve better convergence. It takes a long computational time, so the computational resource is the important factor here.
      (i) Calculates the electric potential.
      (ii) Solves the eigenvalue problem for Kohn-Sham orbitals.
      (iii) Incorporates spin-orbit coupling.
      (iv) Computes the local Green's function and hybridization function.
      (v) Solves the auxiliary impurity problem to obtain the electronic self-energy correction.
      (vi) Calculates the DMFT+DFT valence electronic charge.
      (vii) Adds core states to the DFT charge.
      (viii) Mixes the electronic charge density.
   (c) Then, we calculate the SR-NIEL for the candidate materials [22]. For the energy, we can set the maximum and minimum to 10 to 100 MeV [32].
   (d) Lastly, we can input these NIEL values to the solar radiation degradation software [21] to calculate the EOL performance, after setting mission parameters.

When we find a material that has a higher EOL than the current commercial PV material, then we have found a potential best candidate(s).

3.2 Computational Advancements

The integration of renewable energy resources, particularly photovoltaic (PV) cells, into power grids is gaining momentum, especially for applications in space. The unique challenges posed by the space environment necessitate advancements in materials and computational methods to optimize energy production from PV cells. Below are the computational advancements and optimization strategies relevant to your approach of discovering new materials for PV cells suitable for space applications.

3.2.1 Machine Learning for Material Discovery

Utilizing machine learning (ML) to narrow down the search space for candidate materials is a significant advancement. Supervised ML models can be trained on datasets such as JARVIS, which contains extensive material properties. This allows for efficient identification of suitable and unsuitable candidates by analyzing complex patterns in material characteristics. The application of confusion matrices helps in assessing model performance, providing insights into true positives, true negatives, false positives, and false negatives, which is crucial for refining the model and improving accuracy.

3.2.2 DFT and eDMFT Approaches

The use of Density Functional Theory (DFT) combined with extended Dynamical Mean Field Theory (eDMFT) represents a sophisticated computational approach to evaluate material properties. This method enables the calculation of threshold displacement energy (Ed) and incorporates spin-orbit coupling effects, which are critical for understanding material behavior under radiation exposure. The iterative nature of the DFT and eDMFT loops allows for improved convergence in results, albeit at the cost of increased computational time and resources.

3.2.3 Phonon Calculations

The implementation of phonon calculations using the "frozen phonon" approximation via the Phonopy package is another advancement. This method allows for the generation of displaced atomic structures, facilitating the study of vibrational properties and stability of materials under space conditions. Accurate phonon calculations are essential for predicting how materials will respond to radiation and thermal fluctuations in space.

3.3 Computational Resource Optimization

3.3.1 Efficient Use of Resources

Given the computational intensity of DFT and eDMFT, optimizing resource allocation is vital. Strategies may include:

- **Parallel Computing**: Leveraging high-performance computing (HPC) environments to run multiple simulations simultaneously can significantly reduce computational time.
- **Hybrid Approaches**: Combining ML with quantum methods allows for a more efficient exploration of the material space. By using ML to filter candidates before applying more resource-intensive quantum methods, the overall computational load can be minimized.
- **Adaptive Algorithms**: Implementing adaptive algorithms that can dynamically adjust the computational effort based on the predicted importance of certain materials can lead to more efficient use of resources.

3.3.2 Setting Parameters for Simulations

Carefully setting parameters for simulations, such as energy thresholds for NIEL (Non-Ionizing Energy Loss) calculations, can also optimize computational resources. By focusing on a defined range (e.g., 10 to 100 MeV), the simulations can be tailored to relevant energy levels that are most likely to impact material performance in space environments.

In conclusion, the combination of machine learning for initial candidate screening, advanced computational methods like DFT and eDMFT for detailed property evaluation, and strategic optimization of computational resources forms a robust approach to discovering new materials for PV cells suitable for space applications. This integrated methodology not only addresses the challenges posed by the space environment but also enhances the efficiency of the research process.

4 Future Directions

In moving forward with our research, we must consider the practicality of obtaining or synthesizing the materials identified as potentially optimal, as some may be difficult to source or create. Additionally, it is important to expand our evaluation criteria beyond solar radiation degradation to include other factors affecting PV performance. Our exploration will cover the three main categories of PV technologies: wafer-based cells (e.g., traditional crystalline Si and III-V semiconductors), commercial thin-film cells (e.g., amorphous Si, CdTe, and CIGS), and emerging thin-film technologies such as perovskite, organic, and quantum dot solar cells [14].

We also plan to leverage machine learning to predict key PV parameters [33], further refining our materials discovery process. An important aspect of our ongoing work will involve measuring the efficiency of our pipeline; we need to establish metrics that compare our approach against existing methodologies beyond just end-of-life (EOL) performance. This also ties into the improvement of our training sets, where more robust criteria will be established for determining material suitability. Experimental validation of our simulation results will be crucial, alongside efforts to identify the key characteristics that influence material suitability with minimal properties or features. Our work will continue to expand our list of materials used or experimented with in space PV applications.

Despite encountering technical issues with running our quantum methods, we are committed to resolving these challenges, including requesting additional computational resources. Lastly, we will validate our model's accuracy by cross-referencing with materials from the Jarvis database, employing an empirical approach that builds on existing knowledge of semiconductor suitability for quantum technologies [34].

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