

# Optimizing Materials Discovery for Photovoltaics (PV) in Space

Entangled Energy.

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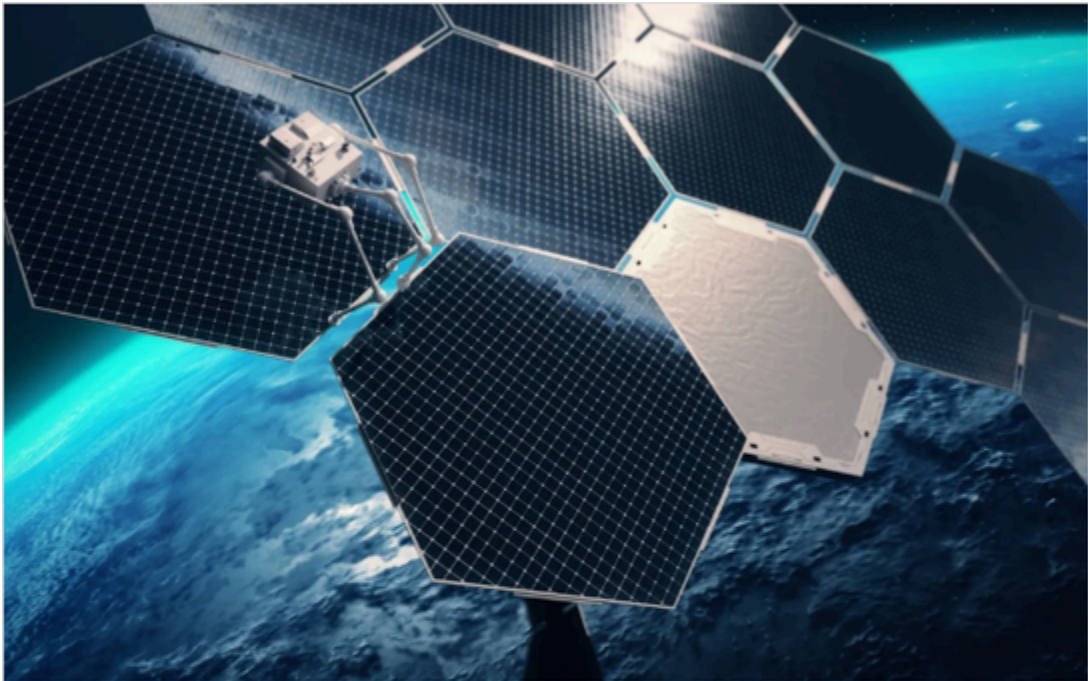
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## International Space Station Facts and Figures

**International Space Station Facts** An international partnership of five space agencies from 15 countries operates the International Space Station. [Learn more](#)

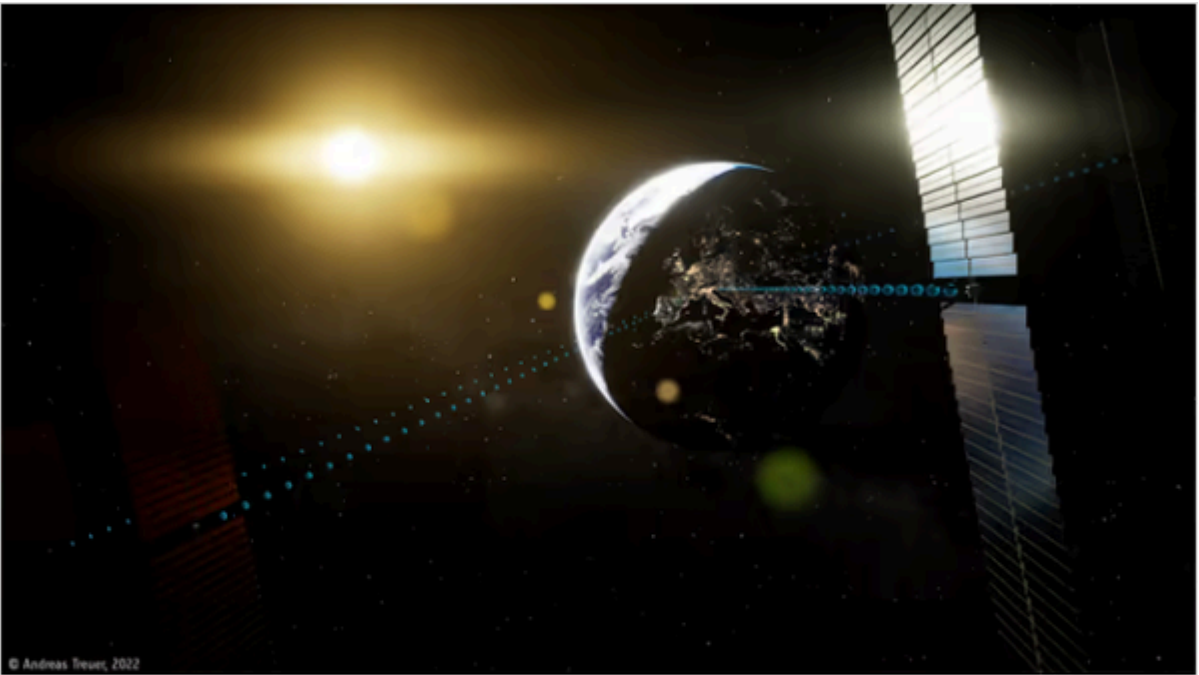
NASA / May 23, 2023



## Thales Alenia Space reveals results of ASCEND feasibility study on space data centers

Thales Alenia Space announces the promising results of the ASCEND (Advanced Space Cloud for European Net zero emission and Data sovereignty) feasibility study.

Thales Alenia Space / Jun 27



# SOLARIS

To prepare Europe for future decision making on Space-Based Solar Power, ESA has kicked-off a preparatory initiative, called SOLARIS, for which funding was approved at the ESA Council at Ministerial Level in...



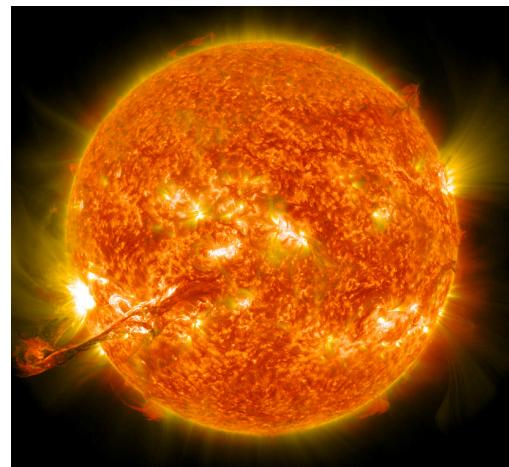
# Space Conditions



**Meteoroids & Space  
Debris**



**Reactive Atomic  
Oxygen**



**Solar Radiation**



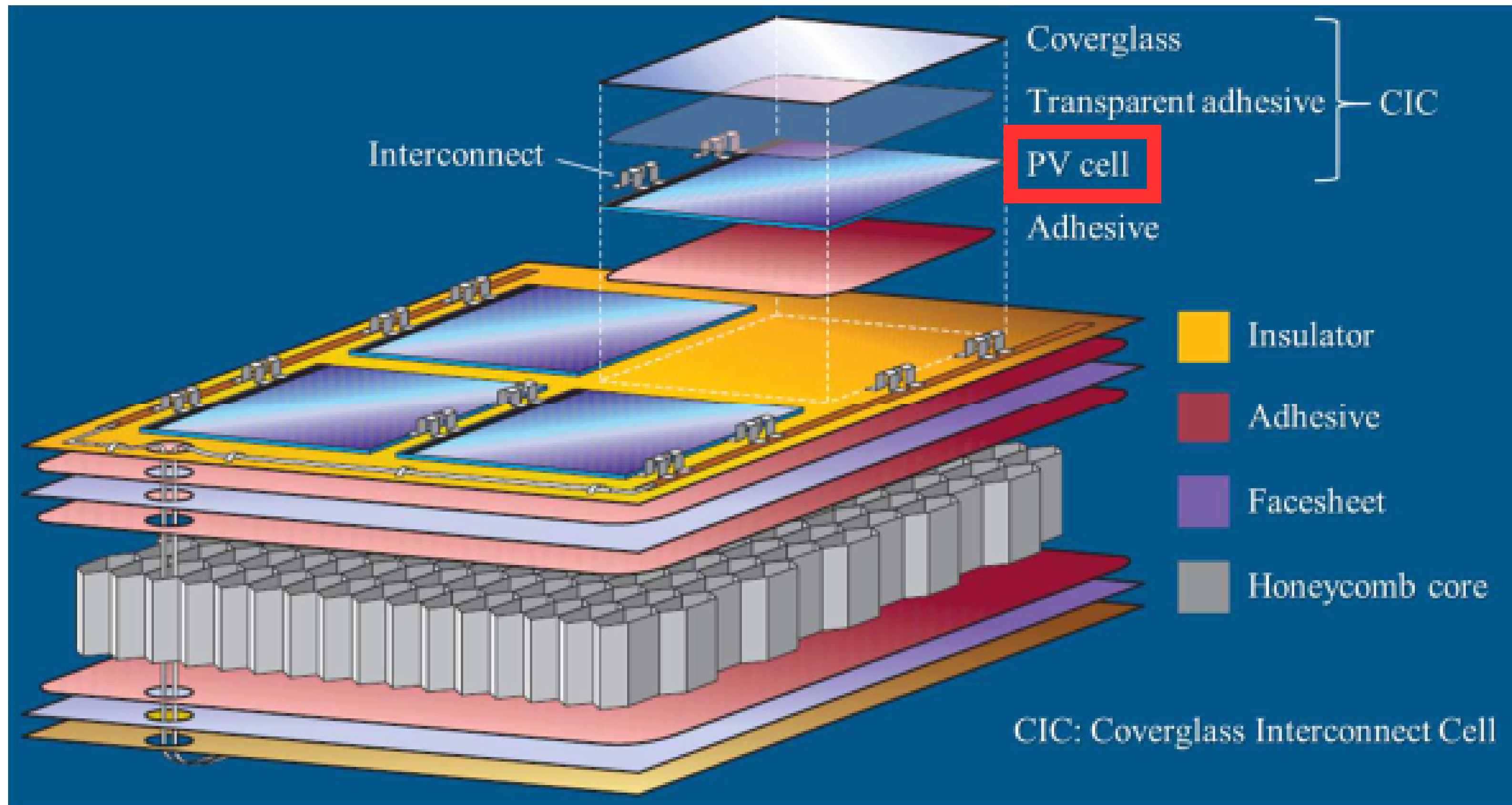


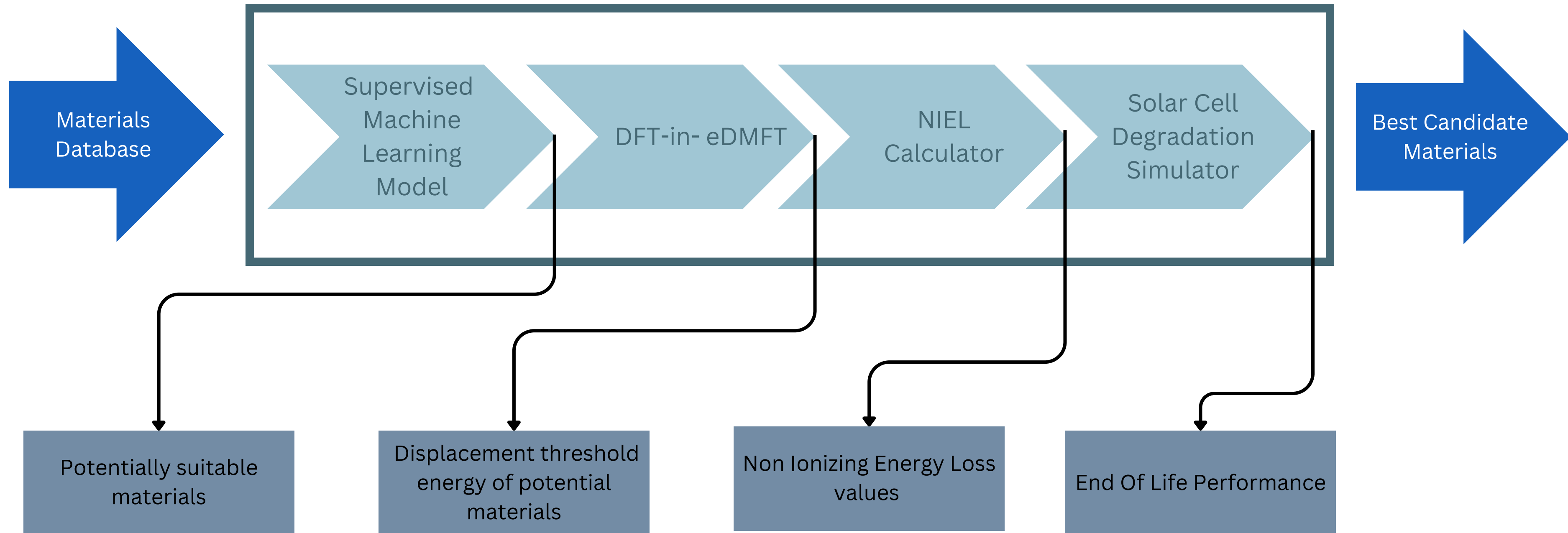
Image adapted from Francis et al., "Thermal Cycling Techniques for Solar Panels," (2005)

# The Problem

There are many materials,  
&

It is expensive to run experiments.

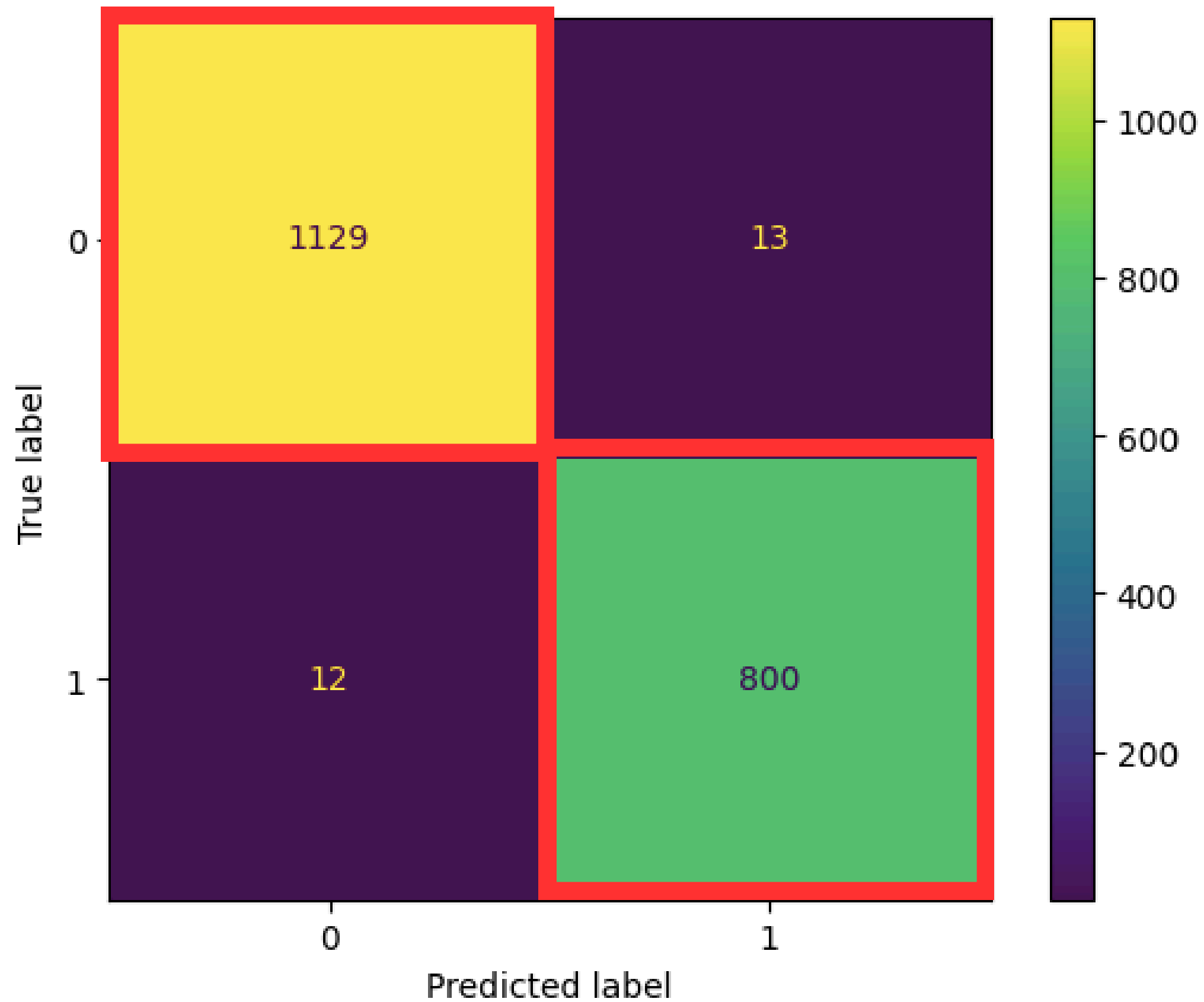
# Our Solution



# Results

formula	predictions
NaLiO	0
Sb4I2O5	0
InBi	0
CaAsH5O6	0
Ag3P11	1
...	...
Cr4InCuSe8	0
YWN3	1
TiPbO3	1

# Results





# Future Directions

- Train on less features
- Consider aspects other than solar radiation
- Develop a pipeline that integrates all the software tools
- Request quantum hardware credits
- Validate our results with experimental results

# Optimizing Materials Discovery for Photovoltaics (PV) in Space

Thank you for listening!



# Appendix

1. Example input and output for DFT in eDMFT
2. NIEL calculator
3. NIEL example output
4. Solar Cell Degradation Simulation example output

# Original structure

GaAs  
F LATTICE,NONEQUIV.ATOMS: 2 216\_F-43m  
MODE OF CALC=RELA unit=ang  
10.866274 10.866274 10.866274 90.000000 90.000000 90.000000  
ATOM -1: X=0.00000000 Y=0.00000000 Z=0.00000000  
MULT= 1 ISPLIT= 8  
Ga NPT= 781 R0=0.00005000 RMT= 2.3400 Z: 31.000  
LOCAL ROT MATRIX: 1.0000000 0.0000000 0.0000000  
0.0000000 1.0000000 0.0000000  
0.0000000 0.0000000 1.0000000  
ATOM 2: X=0.25000000 Y=0.25000000 Z=0.25000000  
MULT= 1 ISPLIT= 8  
As NPT= 781 R0=0.00005000 RMT= 2.3400 Z: 33.000  
LOCAL ROT MATRIX: 0.0000000 0.0000000 0.0000000  
0.0000000 0.0000000 0.0000000  
0.0000000 0.0000000 0.0000000  
0 NUMBER OF SYMMETRY OPERATIONS

# Displaced structure

displacements:  
- atom: 1  
displacement:  
[ 0.02000000000000000, 0.0000000000000000, 0.0000000000000000 ]  
- atom: 1  
displacement:  
[ -0.02000000000000000, -0.0000000000000000, -0.0000000000000000 ]  
- atom: 9  
displacement:  
[ 0.02000000000000000, 0.0000000000000000, 0.0000000000000000 ]  
- atom: 9  
displacement:  
[ -0.02000000000000000, -0.0000000000000000, -0.0000000000000000 ]

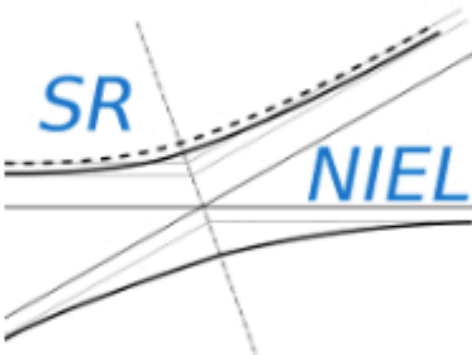
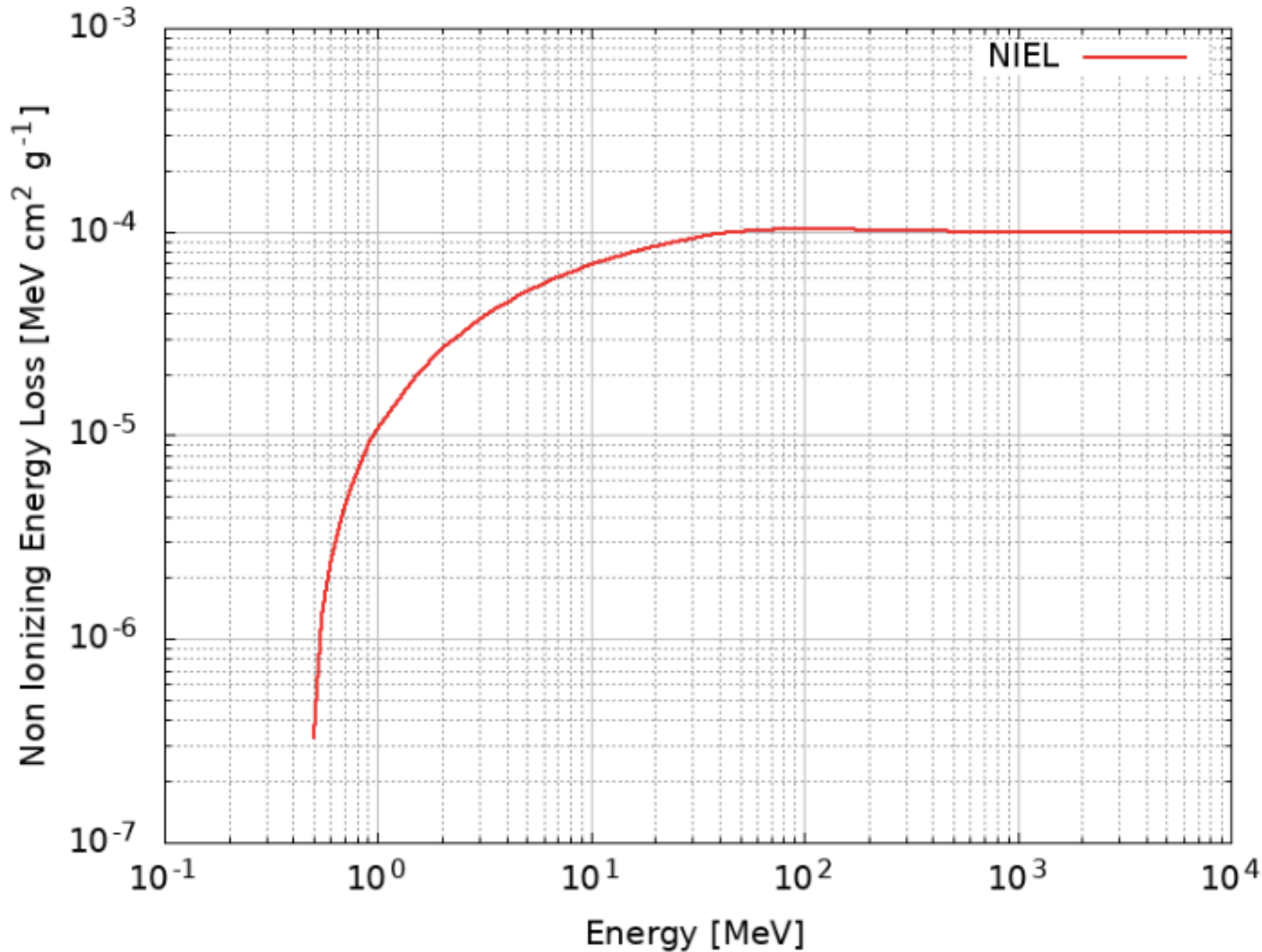
# Electrons NIEL Calculator

Form Factor Model:	Exponential	
Target Materials		
Target Selection:	User Defined	
N° Elements:	2	
Target Material Z	Stoichiometric Index or Element Fraction	Displacement Threshold Energy [eV] *
31:Ga	1	21.5
33:As	1	21.5
NIEL Energy ranges		
Minimum Energy:	0.1 [MeV]	
Maximum Energy:	10000 [MeV]	
Additional Energies (optional):	<div></div> [MeV]	
Dose Imparted for		
Particle Fluence:	1 [cm <sup>-2</sup> ]	
CALCULATE		

SR (screened relativistic) NIEL (non ionizing energy loss) Calculator

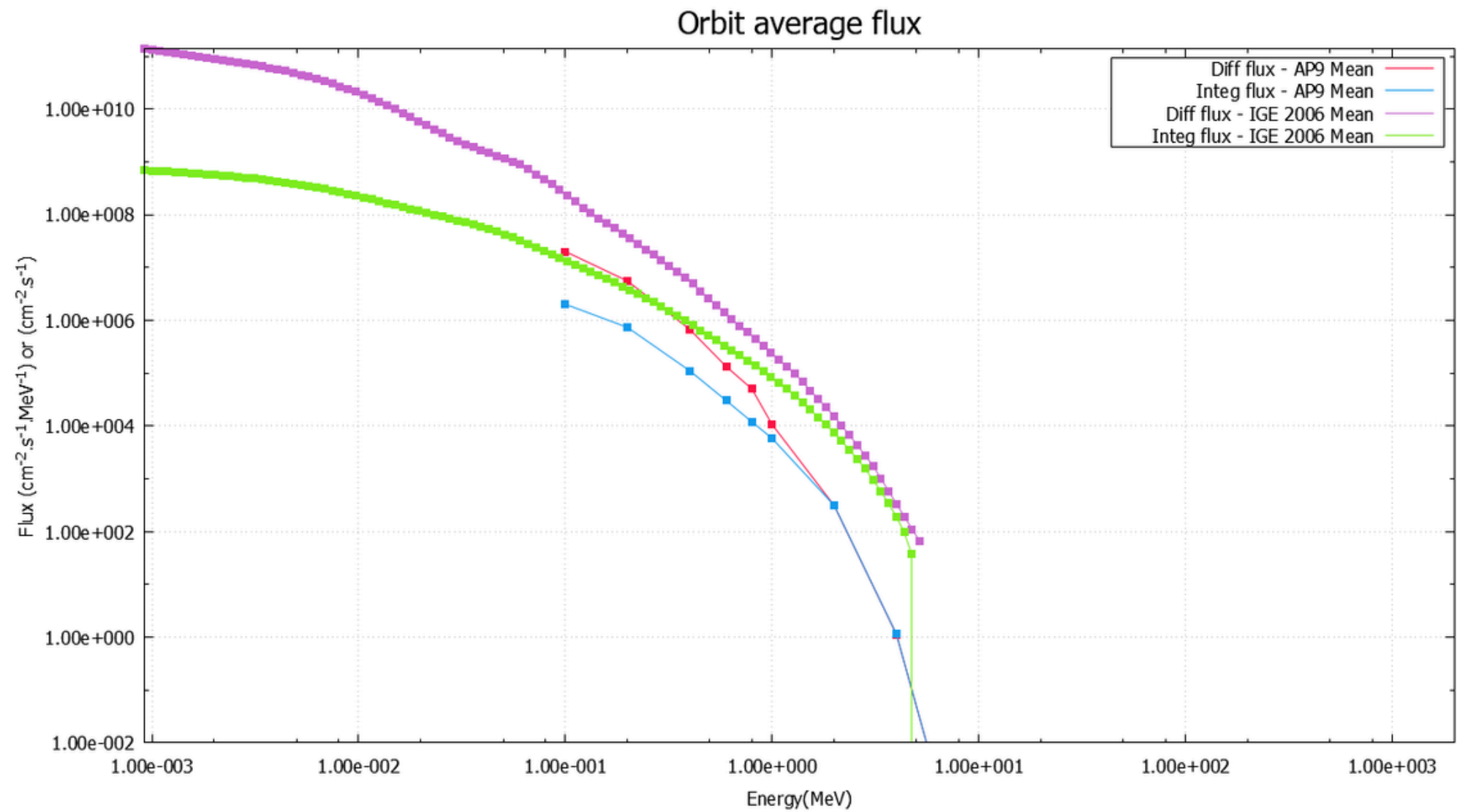
Electrons: SR-NIEL – 7 ver. 10.16 - 26.April.2024

Input Parameters
Electrons in GaAs
Displacement Threshold Energies [eV]: 21.50; 21.50;
Minimum Energy [MeV]: 1.0e-01
Maximum Energy [MeV]: 1.0e+04
Form Factor Model : Exponential
Particle Fluence [cm <sup>-2</sup> ]: 1.00e+00



Energy (MeV)	NIEL (MeV cm <sup>2</sup> g <sup>-1</sup> )	NIEL Dose* (MeV g <sup>-1</sup> )	NIEL Dose* (Gy)
1.0000e-01	0.0000e+00	0.0000e+00	0.0000e+00
1.5000e-01	0.0000e+00	0.0000e+00	0.0000e+00
2.0000e-01	0.0000e+00	0.0000e+00	0.0000e+00
2.5000e-01	0.0000e+00	0.0000e+00	0.0000e+00
3.0000e-01	0.0000e+00	0.0000e+00	0.0000e+00
3.5000e-01	0.0000e+00	0.0000e+00	0.0000e+00
4.0000e-01	0.0000e+00	0.0000e+00	0.0000e+00
4.5000e-01	0.0000e+00	0.0000e+00	0.0000e+00
5.0000e-01	3.2584e-07	3.2584e-07	5.2217e-17
5.5000e-01	1.2643e-06	1.2643e-06	2.0260e-16
6.0000e-01	2.2821e-06	2.2821e-06	3.6572e-16
6.5000e-01	3.3430e-06	3.3430e-06	5.3574e-16
7.0000e-01	4.4237e-06	4.4237e-06	7.0893e-16
7.5000e-01	5.5089e-06	5.5089e-06	8.8283e-16
8.0000e-01	6.5884e-06	6.5884e-06	1.0558e-15
8.5000e-01	7.6555e-06	7.6555e-06	1.2268e-15
9.0000e-01	8.7057e-06	8.7057e-06	1.3951e-15
9.5000e-01	9.7361e-06	9.7361e-06	1.5603e-15
1.0000e+00	1.0745e-05	1.0745e-05	1.7220e-15
1.5000e+00	1.9604e-05	1.9604e-05	3.1416e-15
2.0000e+00	2.6587e-05	2.6587e-05	4.2608e-15
2.5000e+00	3.2259e-05	3.2259e-05	5.1697e-15
3.0000e+00	3.7003e-05	3.7003e-05	5.9300e-15
3.5000e+00	4.1064e-05	4.1064e-05	6.5808e-15
4.0000e+00	4.4604e-05	4.4604e-05	7.1480e-15
4.5000e+00	4.7724e-05	4.7724e-05	7.6407e-15





#===== Calculation Parameters =====

# Cell Technology: GaAs/Ge 1J

# NIEL Material: GaAs

# Electrons C: 3.630e-01

# Dx: 6.900e+09 MeV/g

# n: 1.647e+00

# Protons C: 2.904e-01

# Dx: 1.100e+09 MeV/g

# n: 1.000e+00

# Back Shielding: Infinite

# Coverglass || Displacement

# Thickness || Damage Dose

# (um) || (MeV/g)

# || Electrons || Protons || Total

#-----||-----||-----||-----

1.000e+02 2.734e+08 2.859e+09 3.133e+09

EOL  
Performance  
(%%)  
8.300e+01

#----- INPUT ISOTROPIC FLUENCES -----#

# PROTONS FLUENCES

# Energy DIFFERENTIAL FLUENCE INTEGRAL FLUENCE

# MeV MeV-1.cm-2 cm-2

0.100 9.459e+15 9.501e+14

0.200 2.612e+15 3.465e+14

0.400 3.171e+14 5.366e+13

0.600 6.283e+13 1.566e+13

0.800 2.361e+13 7.017e+12

1.000 5.083e+12 4.150e+12

1.000 5.748e+12 4.148e+12

2.000 4.433e+11 9.951e+11

3.000 1.895e+11 6.403e+11

4.000 1.085e+11 4.921e+11

5.000 7.145e+10 4.032e+11

6.000 5.241e+10 3.402e+11

7.000 4.031e+10 2.917e+11