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Optimizing Materials Discovery for Photovoltaics (PV) in Space

Entangled Energy
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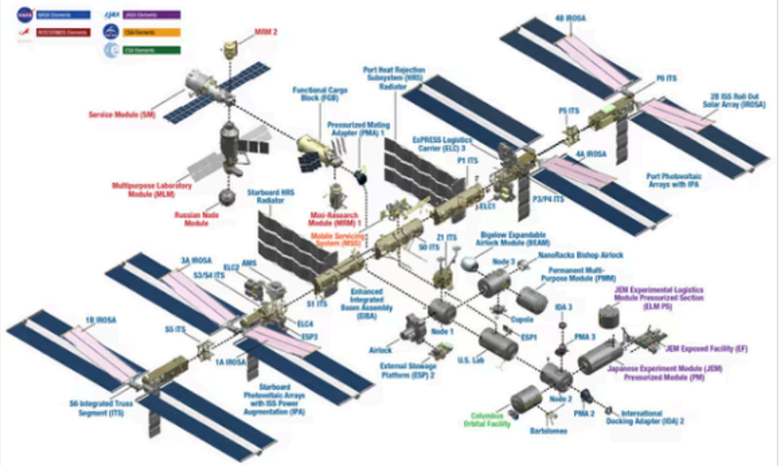
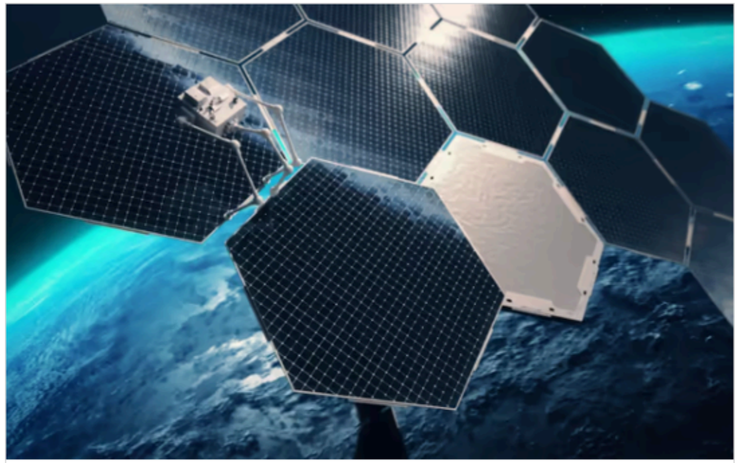
Womanium Quantum+AI Project 2024



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

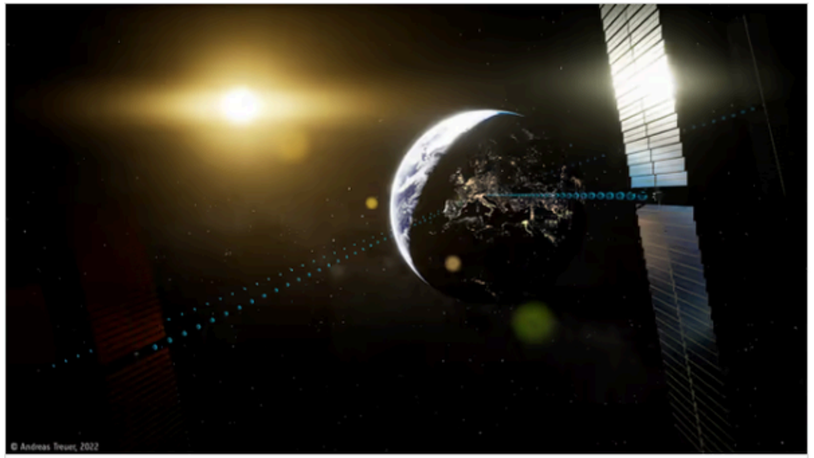
NASA / May 23, 2023



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

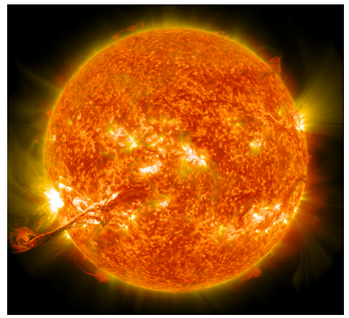
To prepare Europe for future decision making on Space-Based Solar Power, ESA has kicked-off a preparatory initiative, called SOLARIS, for which funding was approved at the ESA Council at Ministerial Level in...

esa

Space Conditions

Meteoroids & Space Debris

Reactive Atomic Oxygen



Solar Radiation

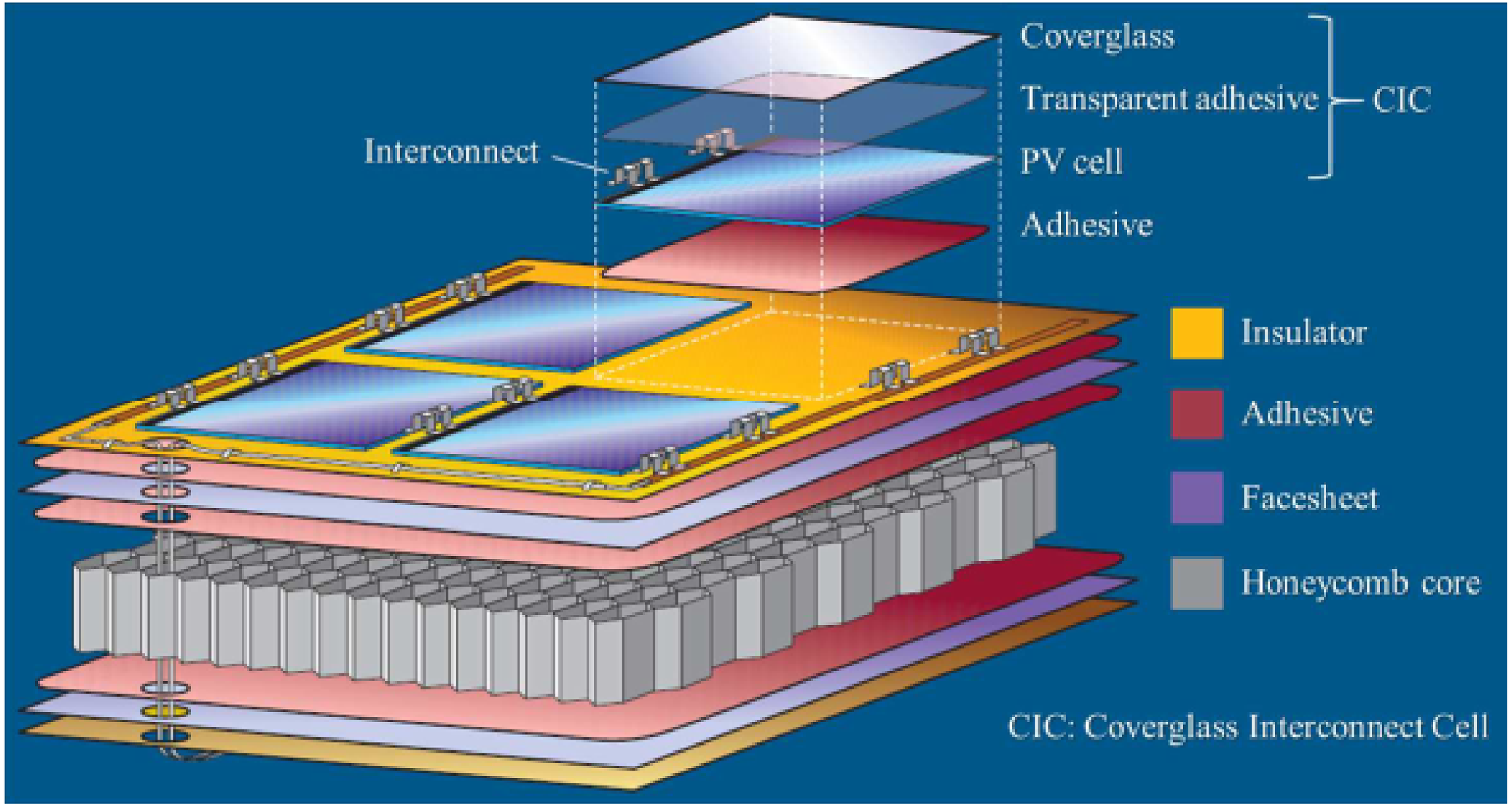


Image adapted from Francis et al.,"Thermal Cycling Techniques for Solar Panels," (2005)

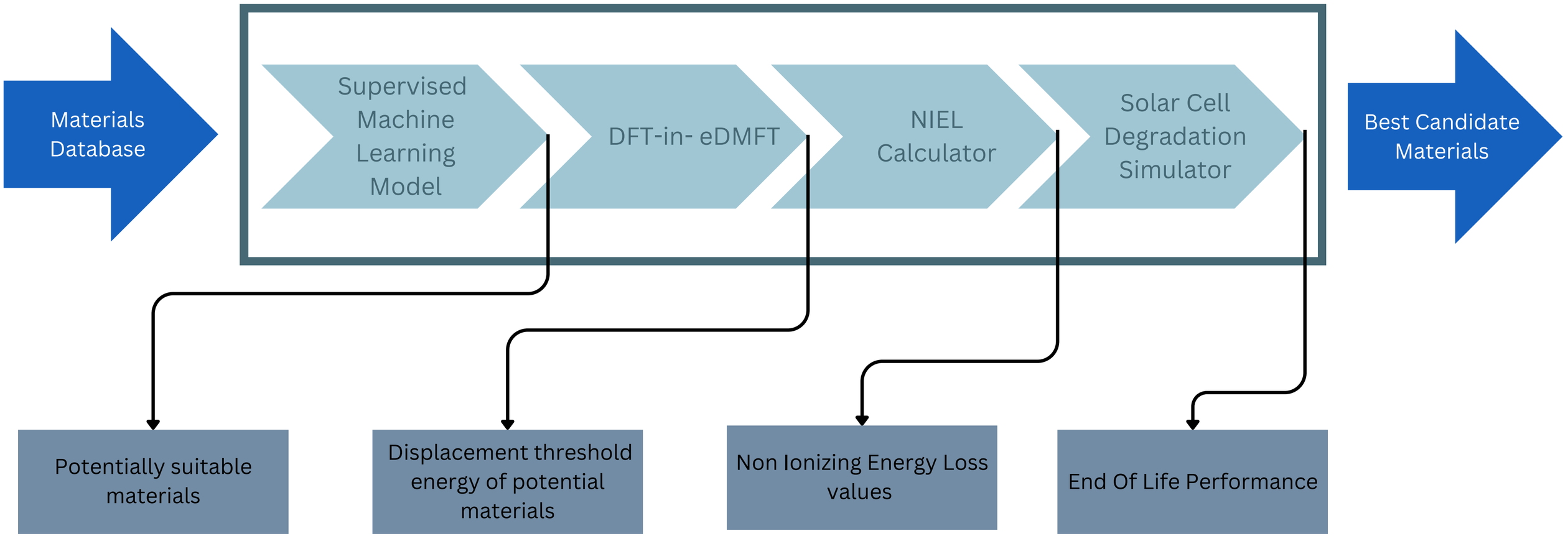
The Problem

There are **many** materials,

&

It is **expensive** to run experiments.

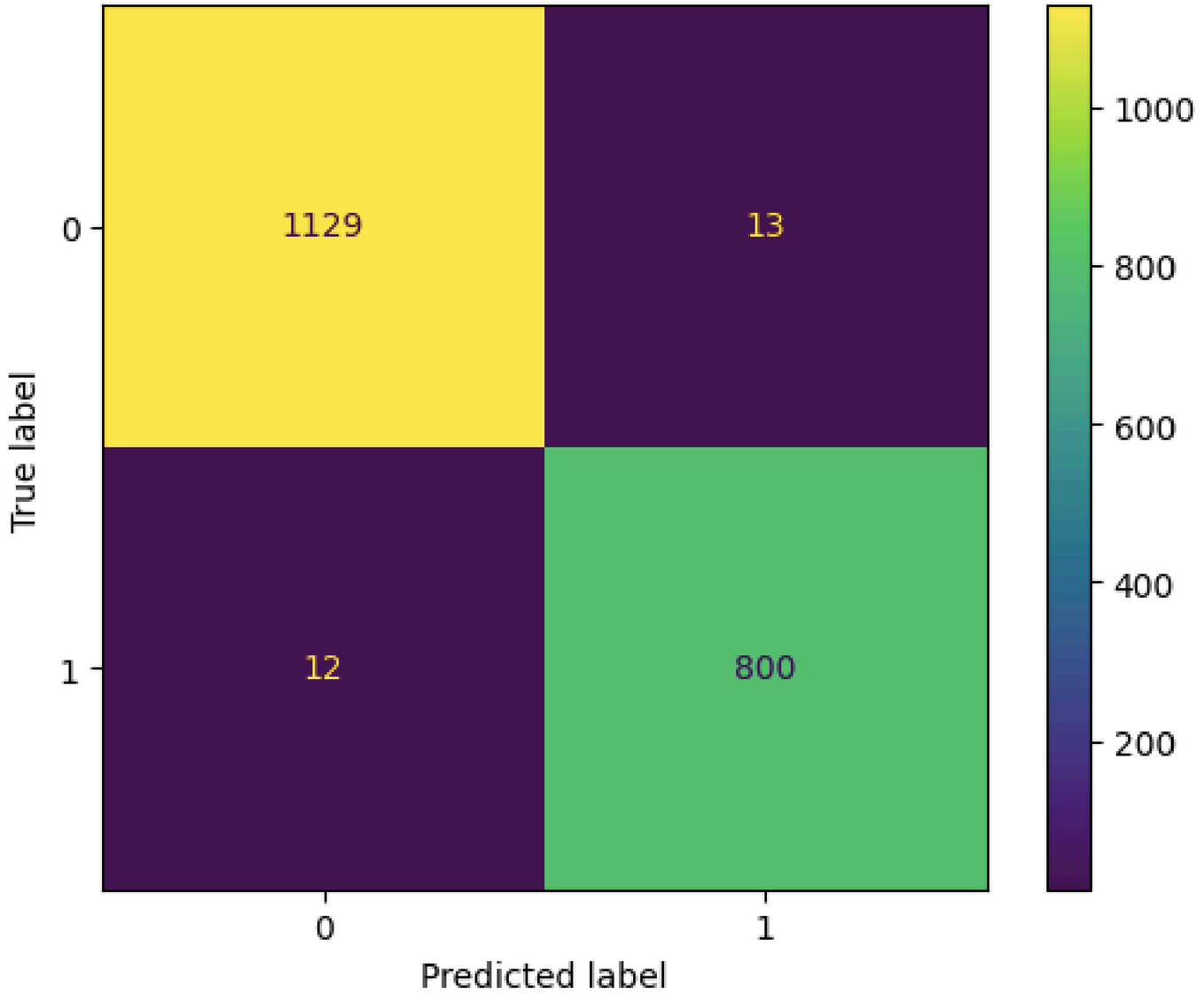
Our Solution



Results

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

Results


1129
13
12
800
0
1
True label
0
1
Predicted label
1000
800
600
400
200

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

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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:
    [   0.0200000000000000,  0.0000000000000000,  0.0000000000000000 ]
- atom:    1
  displacement:
    [  -0.0200000000000000, -0.0000000000000000, -0.0000000000000000 ]
- atom:    9
  displacement:
    [   0.0200000000000000,  0.0000000000000000,  0.0000000000000000 ]
- atom:    9
  displacement:
    [  -0.0200000000000000, -0.0000000000000000, -0.0000000000000000 ]
```

Electrons NIEL Calculator

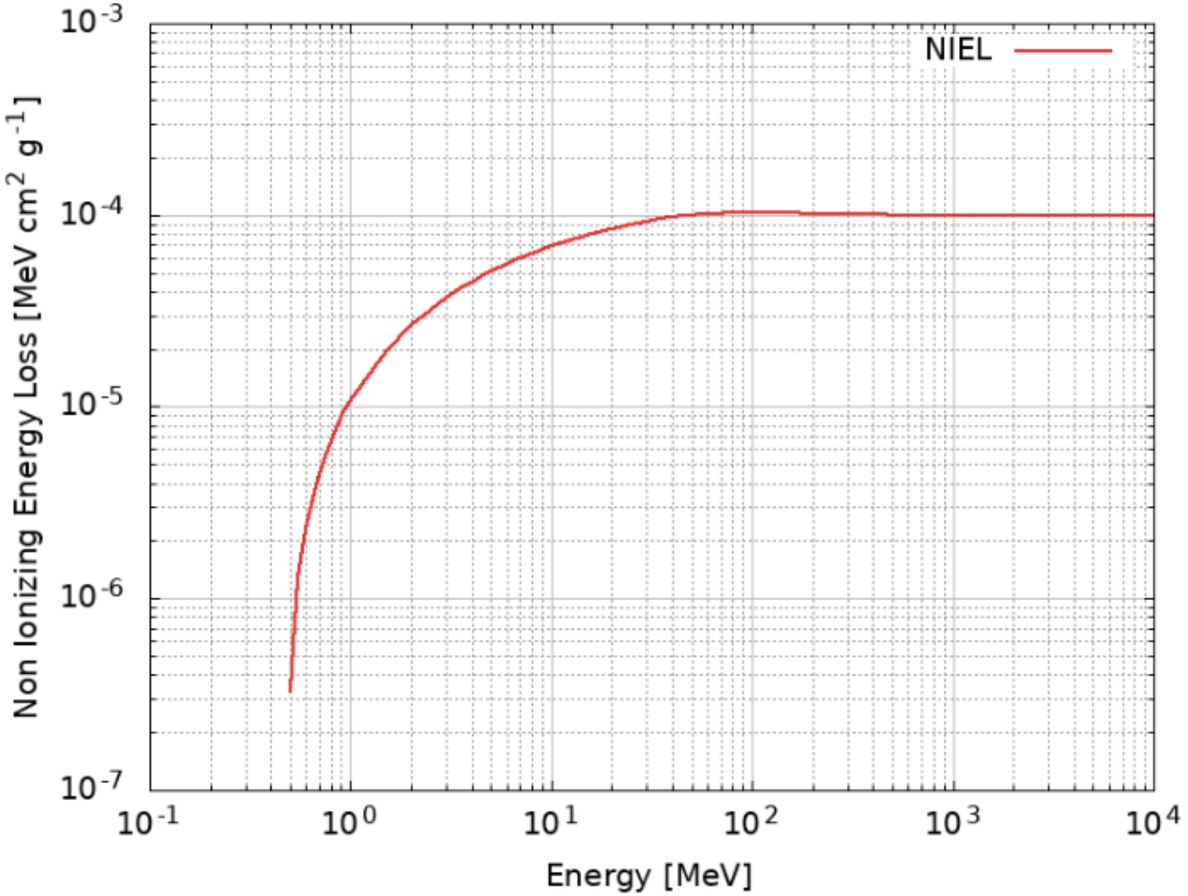
Form Factor Model:	Exponential		
Target Materials			
Target Selection:	User Defined		
N° Elements:	2		
Target Material Z	**Stoichiometric Index or Element Fraction**	**Displacement Threshold Energy [eV]** *	
31:Ga	1	21.5	
33:As	1	21.5	
NIEL Energy ranges			
Minimum Energy:	0.1	[MeV]	
Maximum Energy: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

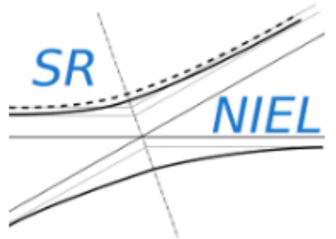
CALCULATE

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

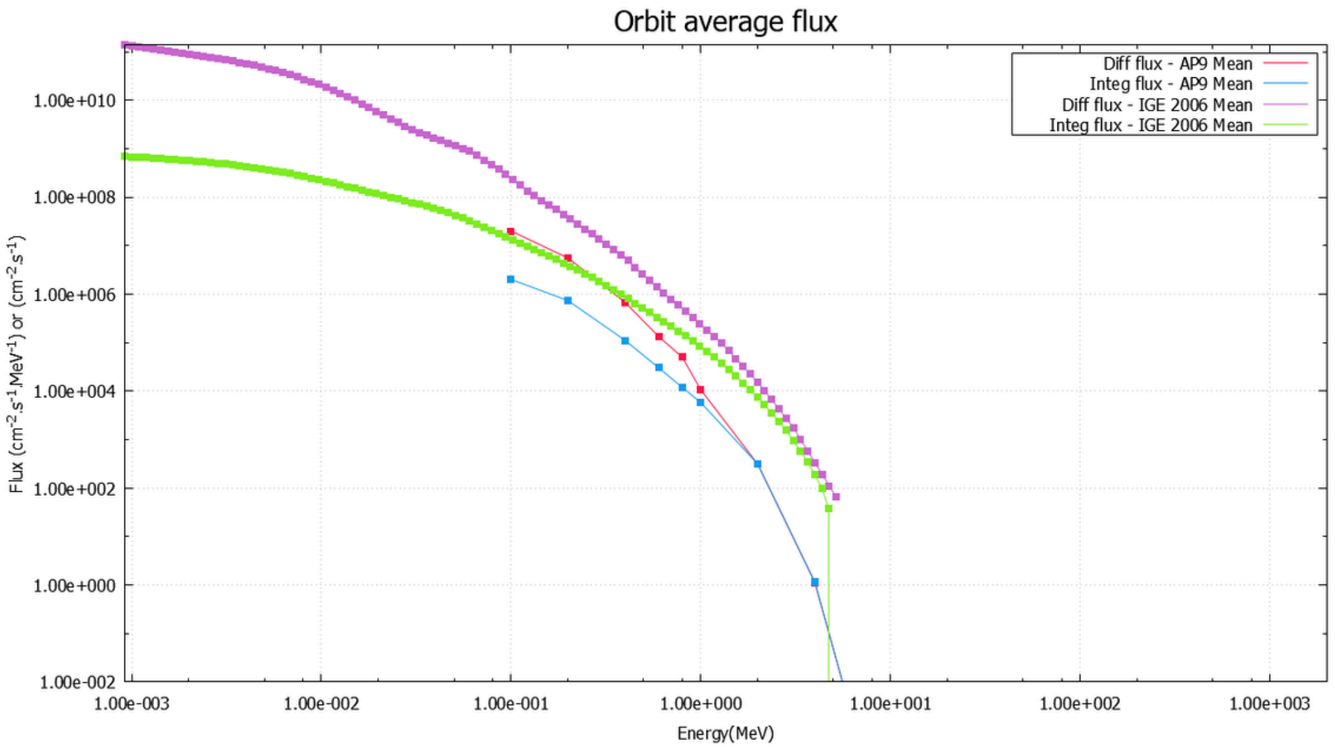
Electrons: SR-NIEL – 7 ver. 10.16 - 26.April.2024

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^{-2}]: 1.00e+00





Energy (MeV)	NIEL (MeV cm^2 g^{-1})	IEL Dose* (MeV g^{-1})	NIEL Dose* (Gy)
1.0000e-01	0.0000e+00	.0000e+00	0.0000e+00
1.5000e-01	0.0000e+00	.0000e+00	0.0000e+00
2.0000e-01	0.0000e+00	.0000e+00	0.0000e+00
2.5000e-01	0.0000e+00	.0000e+00	0.0000e+00
3.0000e-01	0.0000e+00	.0000e+00	0.0000e+00
3.5000e-01	0.0000e+00	.0000e+00	0.0000e+00
4.0000e-01	0.0000e+00	.0000e+00	0.0000e+00
4.5000e-01	0.0000e+00	.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




```
#========== 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                ||      EOL      ||
# Thickness  ||             Damage Dose                 ||  Performance  ||
#     (um)   ||              (MeV/g)                    ||      (%%)     ||
#            || Electrons  |  Protons   |    Total      ||               ||
#------------||------------|------------|---------------||---------------||
  1.000e+02    2.734e+08    2.859e+09    3.133e+09          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     4.034e+10     2.947e+11
```