Exploring NOMAD Entries (hands-on)

FAIRmat tutorial 16
February 26, 2025

Question 1:

How many entries of hexaonal boron nitride (h-BN) are available in NOMAD?

Hints:

- ❑ Use Elements / Formula filter
- ❑ Use Structure / Symmetry filter

Question 2:

What is the range of bandgap of h-BN in NOMAD entries?

Hint:

- ❑ Use Properties -> Electronic filter

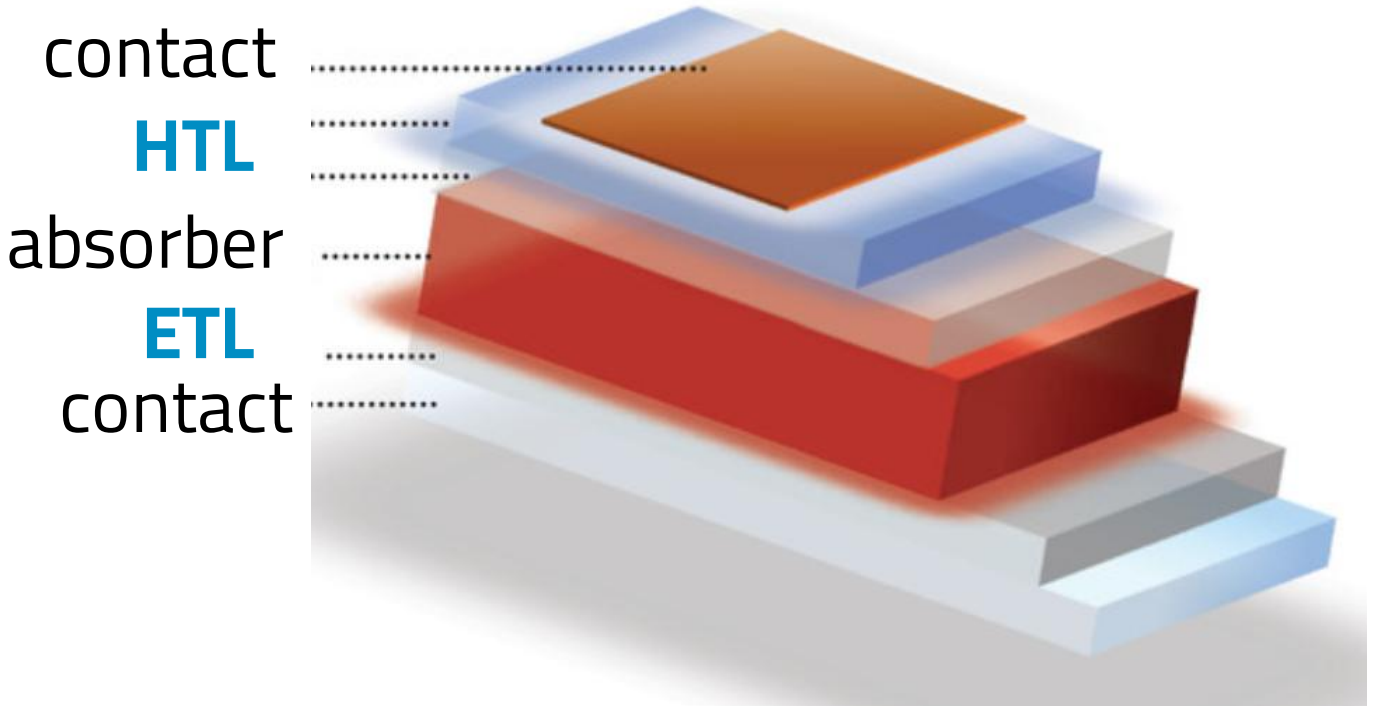
Question 3:

How many entries in NOMAD have calculated bandgap of h-BN between 5.9 eV and 6.5 eV?

Hint:

- ❑ Use the slider or give exact min. and max. values in Properties -> Electronic filter

Example 2: Solar Cells



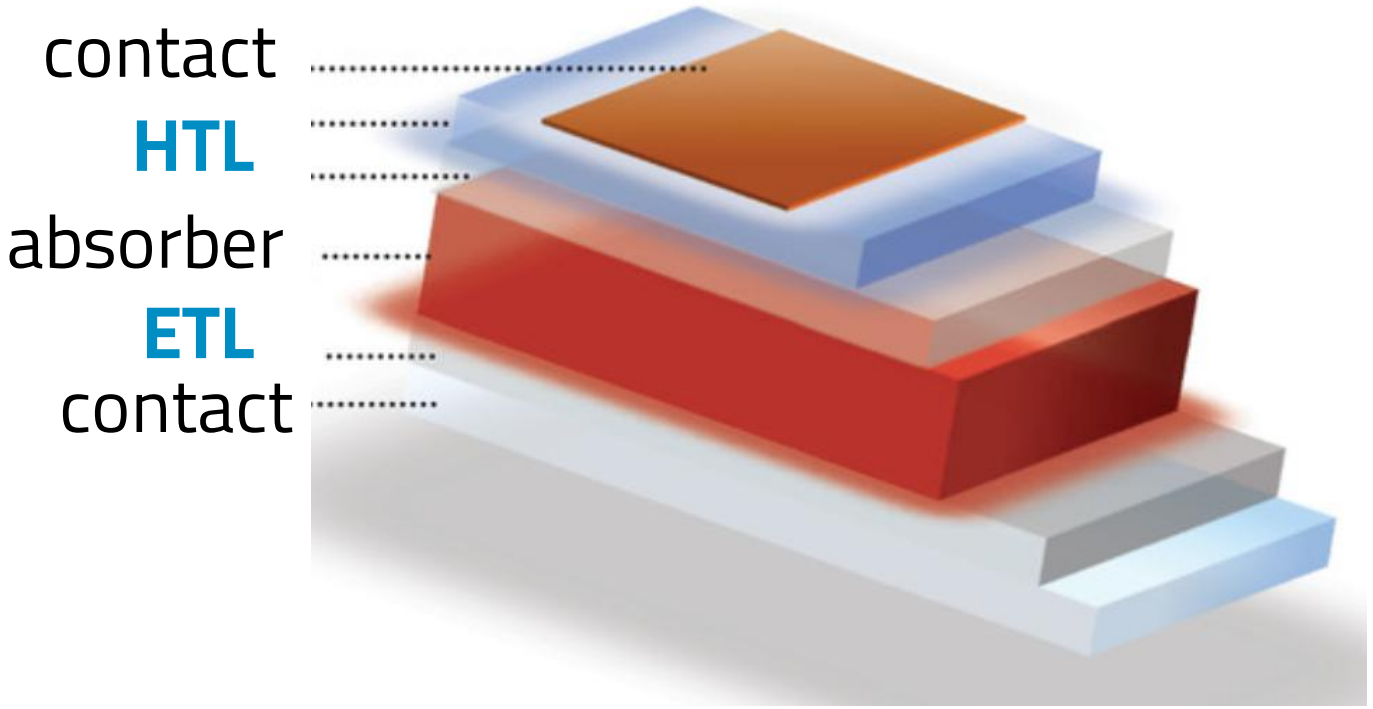
ETL: Electron Transport Layer

HTL: Hole Transport Layer

Example 2: Solar Cells

My device:

contact: Au
HTL: Spiro-OMeTAD ($C_{81}H_{68}N_4O_8$)
Perovskite absorber: CsPbBrI
ETL: TiO_2-c (compact Titanium Dioxide)
contact: FTO (Fluorine-doped Tin Oxide)
Substrate: SLG (Soda Lime Glass)



ETL: Electron Transport Layer

HTL: Hole Transport Layer

Question 1:

How many entries in NOMAD have the elements of the absorber layer (CsPbBrI)?

Question :

How many of those entries include solar cells data with the CsPbBrI as an absorber layer, SpiroOMETAD as HTL and TiO2-c as ETL ?

Hint:

❑ Look Use Cases -> Solar Cells filter

Question 3:

Show the range of reported efficiencies from these entries.

Hint:

- ❑ Use HISTOGRAM widget, for X AXIS start typing “efficiency”

Question 4:

Show an overview of the available entries with info about short circuit current density, efficiency, and open circuit voltage.

Hints:

- ❑ Use SCATTER PLOT widget, for X AXIS start typing “open circuit voltage”, for Y AXIS “efficiency”, for MARKER COLOR “open circuit voltage”