



Discovering One Molecule Out of a Million

-Inverse Design of molecular hole transporting semiconductors tailored for perovskite solar cells

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21/05/2024||| Jianchang Wu||| High Throughput Materials and Devices for PV

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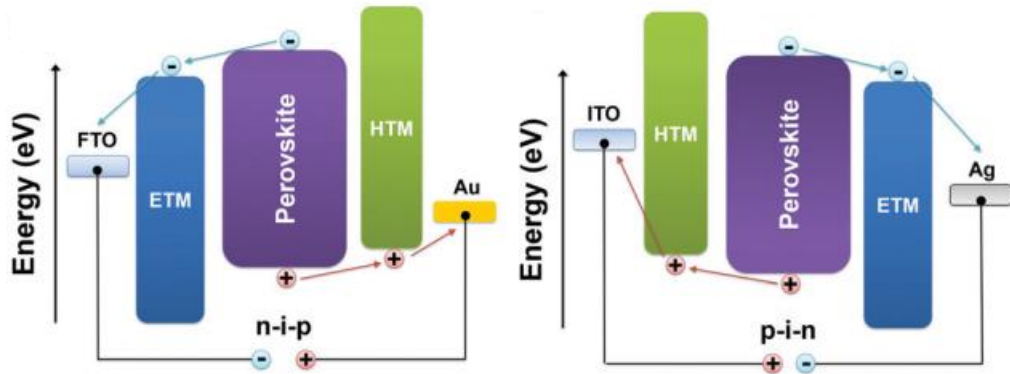
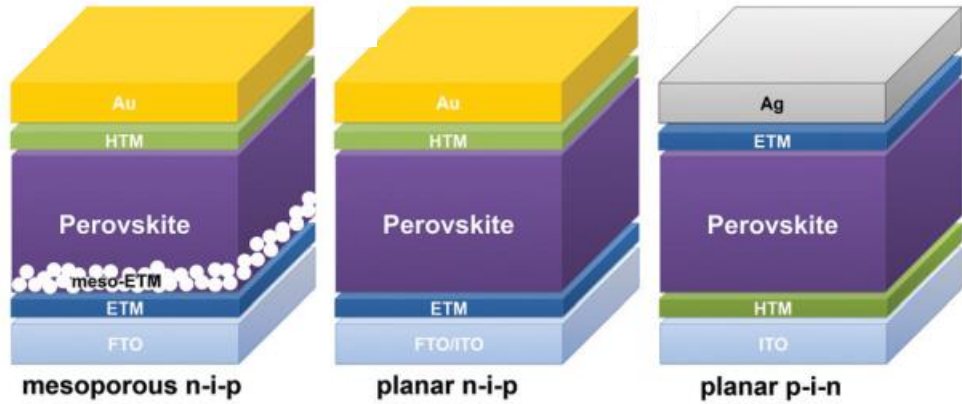
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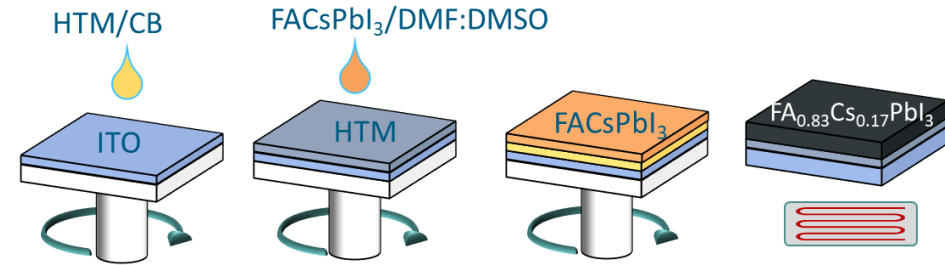
in cooperation with



Background



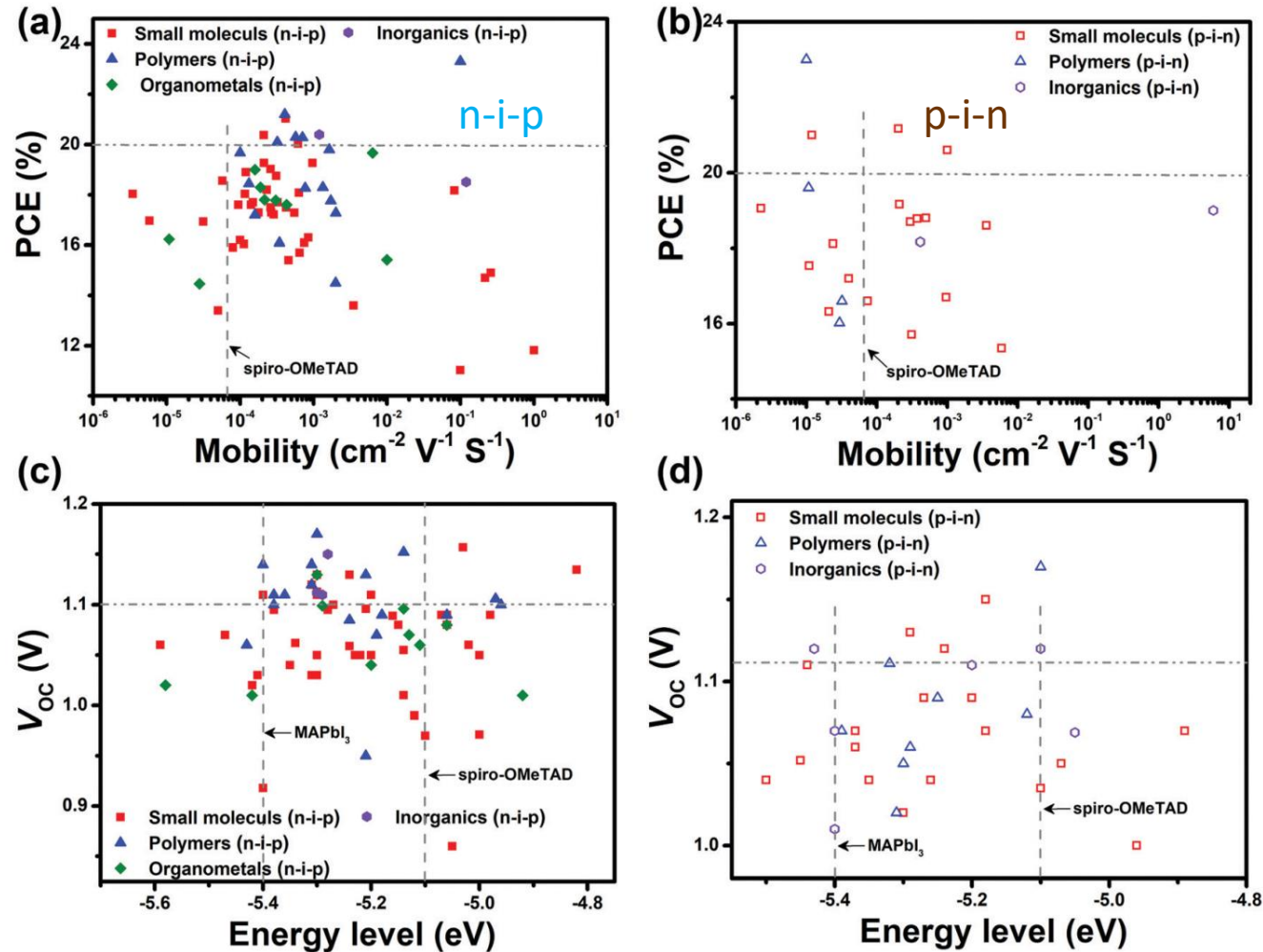
Device fabrication process:



The role of hole transporting material (HTM):

- Perovskite crystallization (pin)
- Charge extraction
- Perovskite defect passivation
- Charge transportation (nip)

Structure-performance relationship



HOMO: General rule

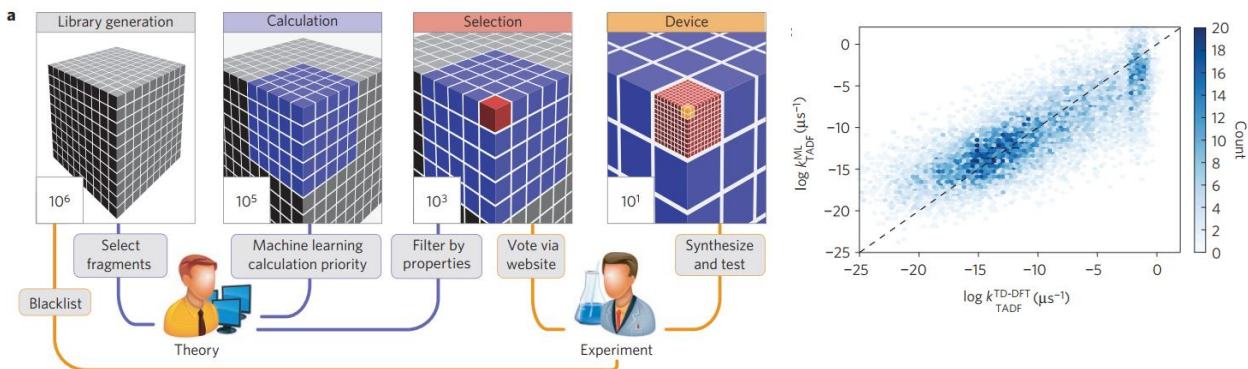
Mobility: Specific rule

How to find more general and hidden rules?

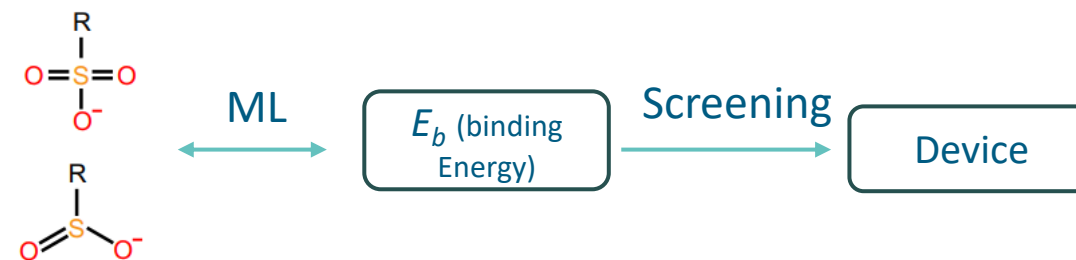
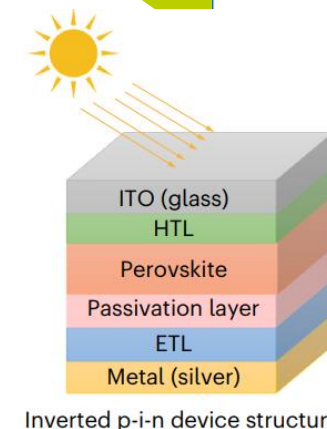
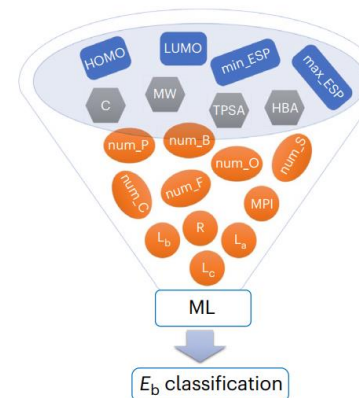
Data: rich and diverse

Machine learning

ML accelerate Material Discovery



- ❑ Link structure to molecular property
- ❑ Screen promising materials for device

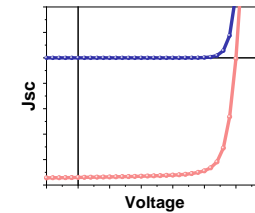
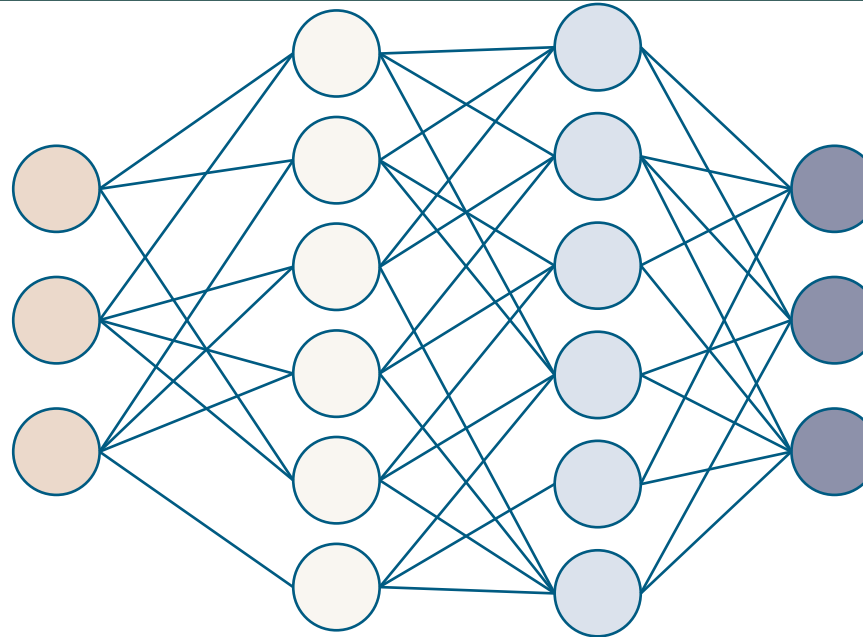
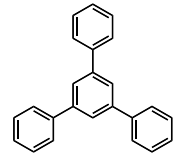


Link the structure to complex device by machine learning



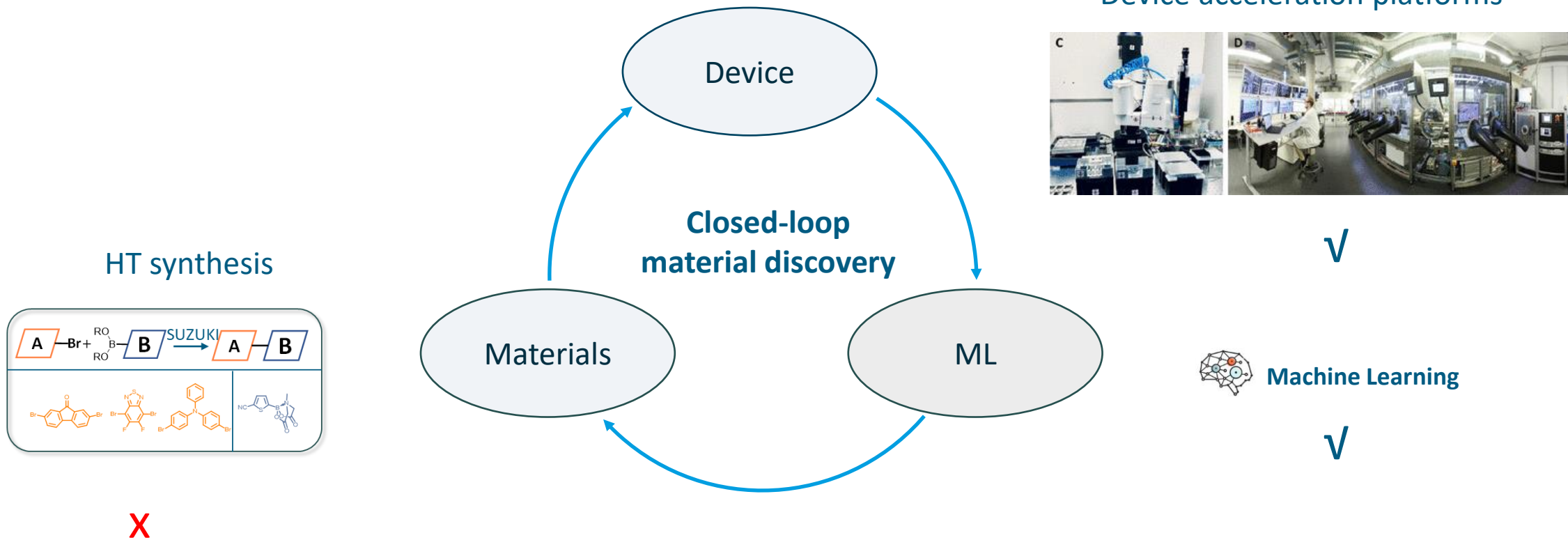
Possible factors:

- **Structure:** aromatic species, conjugated length, active group and D-A effect...
- **HTM Film:** wettability, mobility, HOMO...
- **HTM/PVK:** hole extraction, charge combination, crystal growth...
- **Device:** Voc, Jsc and FF.

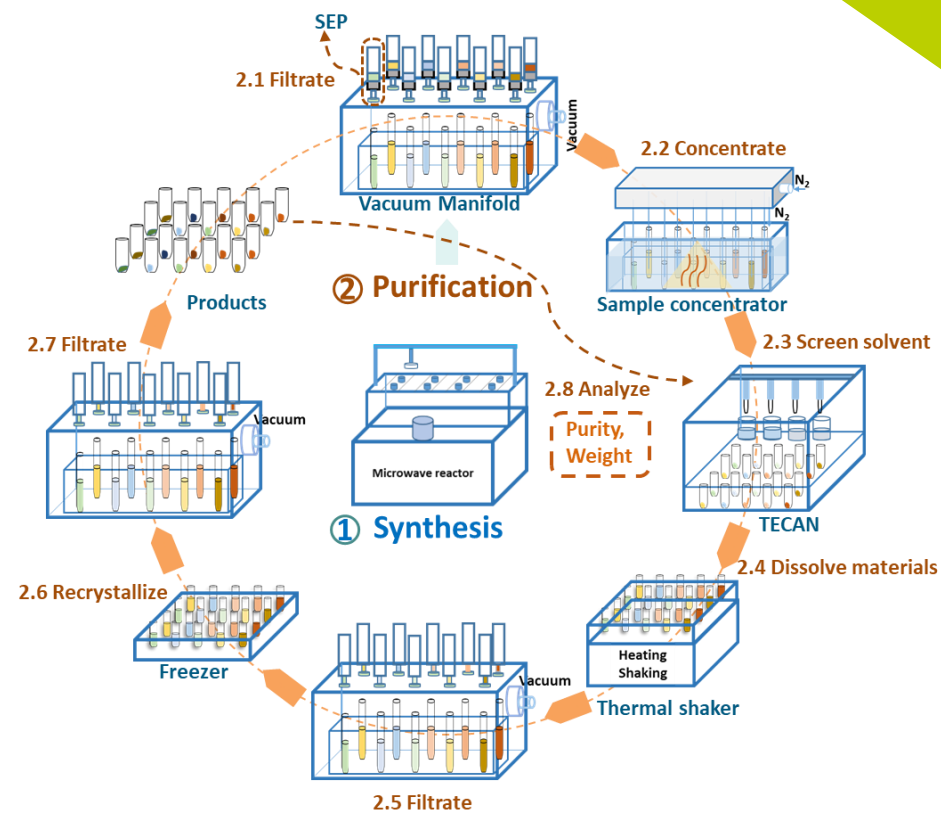
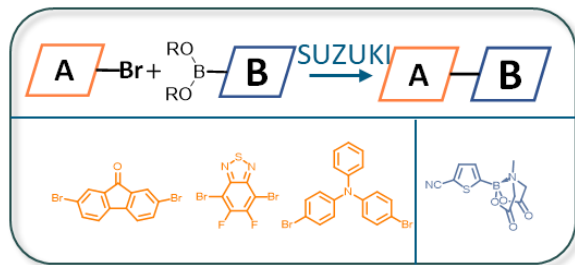


- Complex correlation mechanisms
- Intermediate connectors

Closed-loop material discovery using experimental data

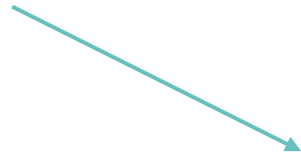


How to do HT purification ?



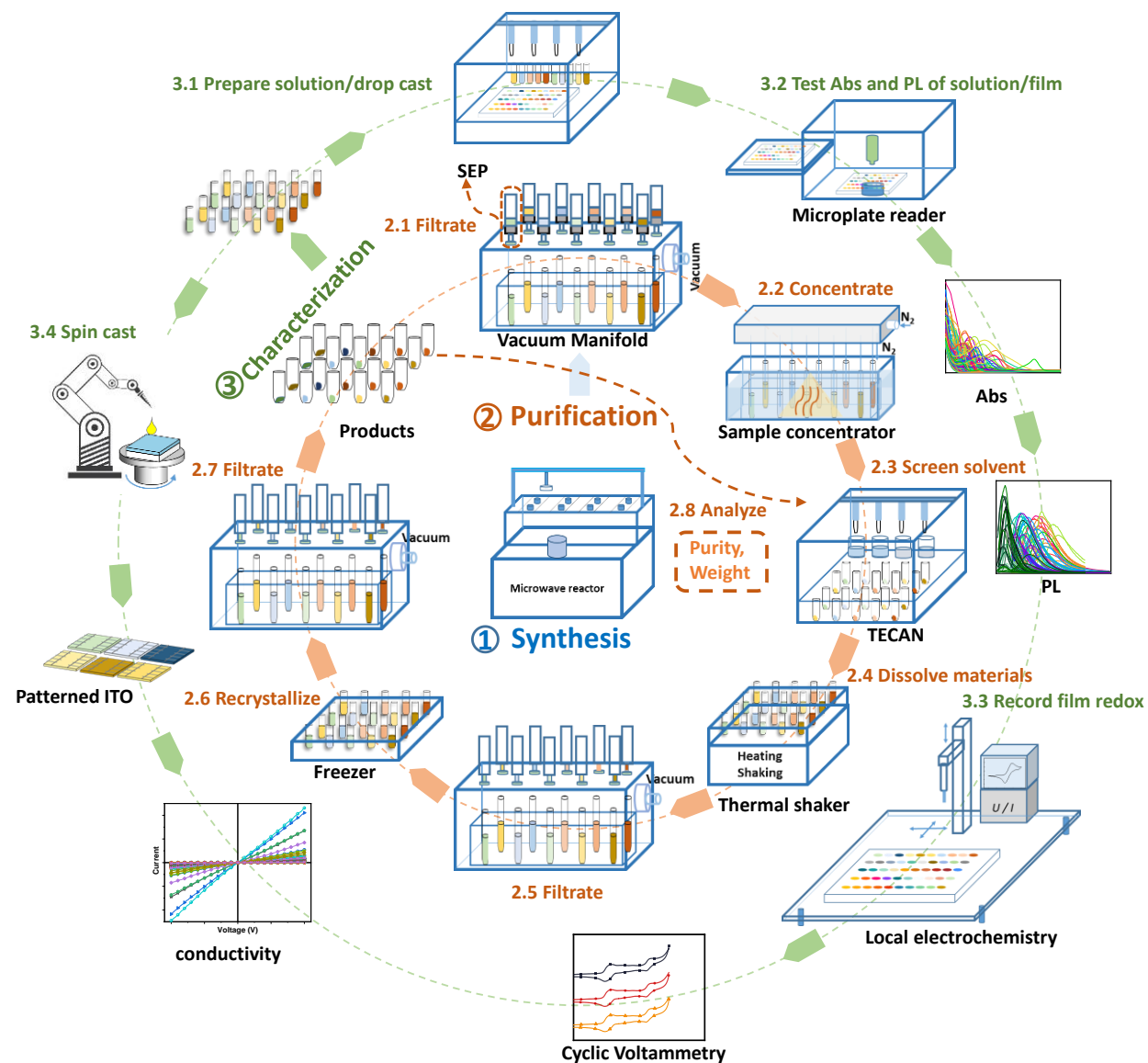
What's in the reaction solution:

- Residual reactants: Pd(OAc)₂, sPhos, K₃PO₄, monomer A, and B
- By products: A-A, B-B, A-A-B...
- Product: A-B



- Water washing and flash chromatography (step 2.1)
- HT reaction condition optimization (high yields)
- DFT calculation and robot assisted recrystallization (steps 2.3-2.7). Highly compatible with device fabrication.

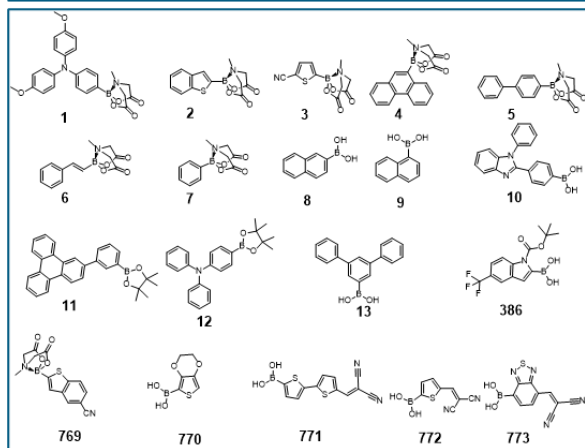
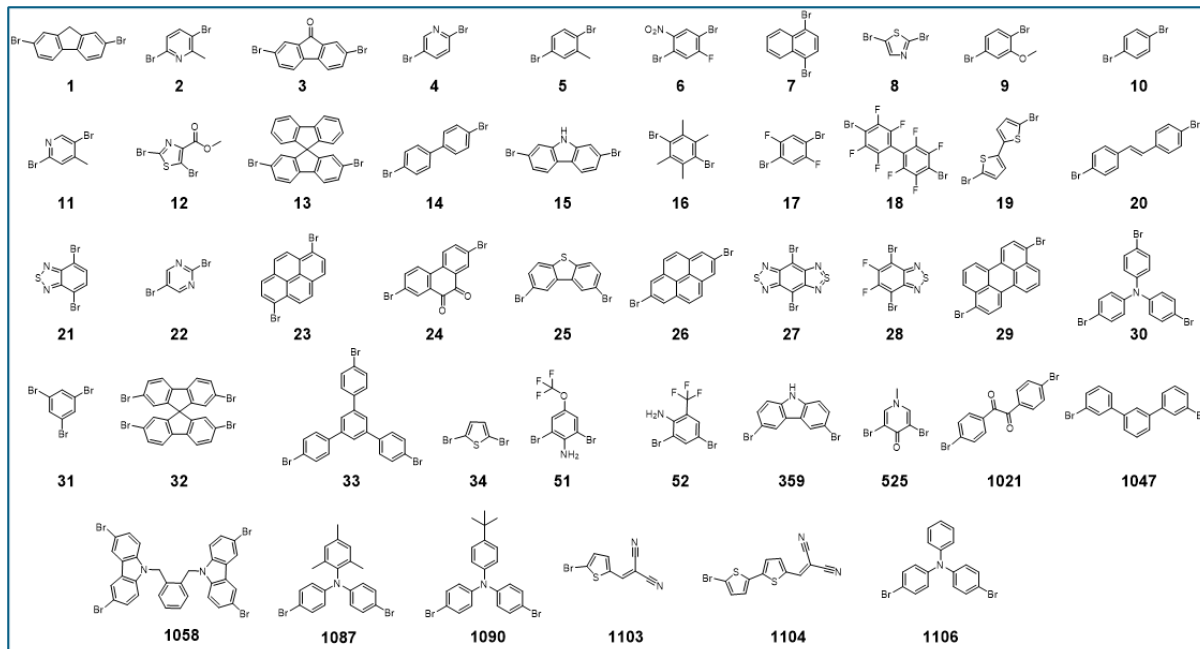
An integrated system built for small-molecule semiconductors



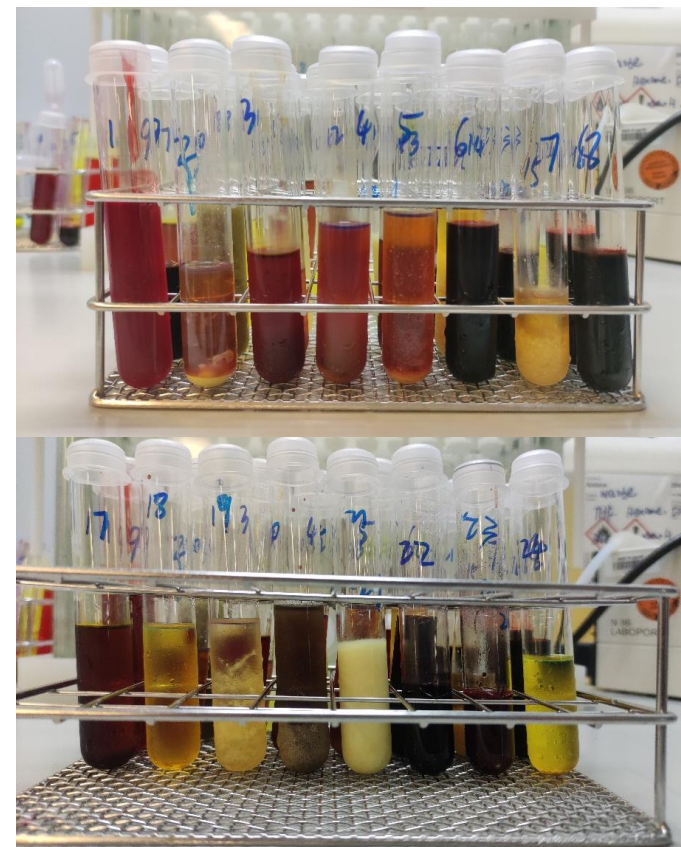
- I. HT reaction and optimization
- II. HT purification: flash chromatography + robotic recrystallization
- III. Sample preparation. Drop casting and spincoating to make films.
- IV. Characterizations: UV-vis, PL, electrochemistry, and conductivity

Recrystallization

Monomers for synthesis



Recrystallization

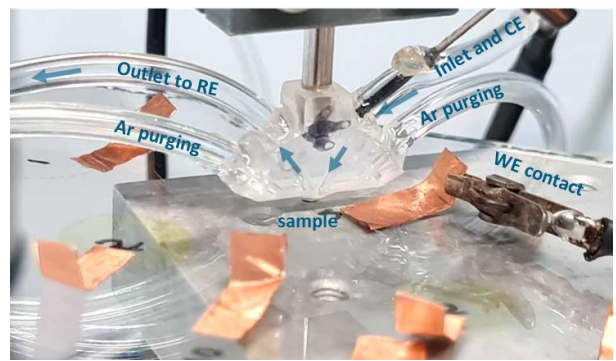
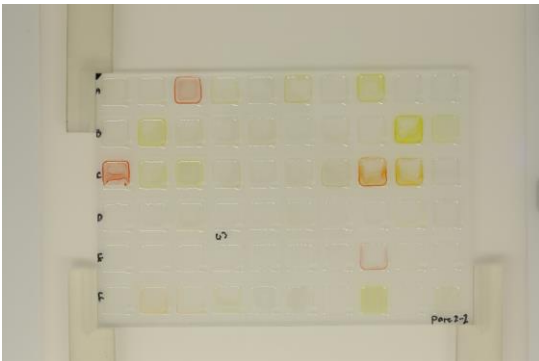


HT Optical and Electrical Characterization

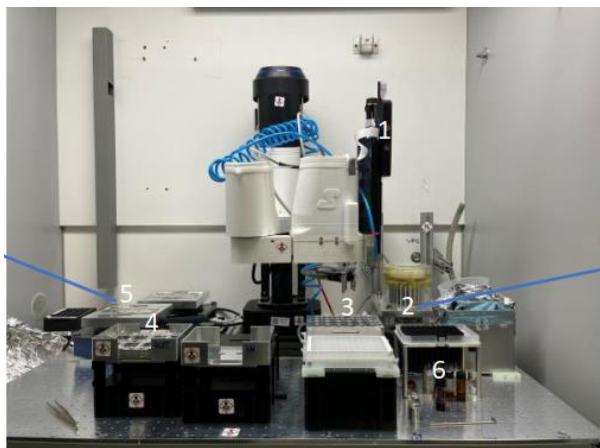
UV-vis and PL



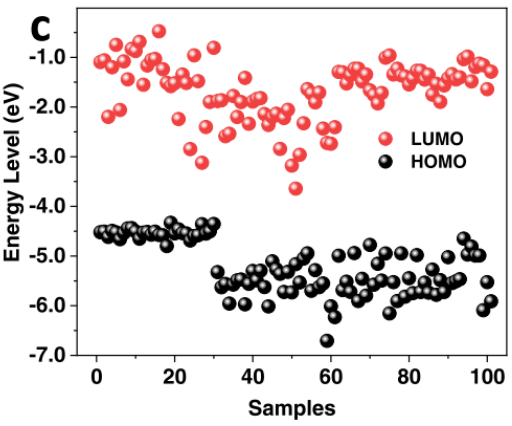
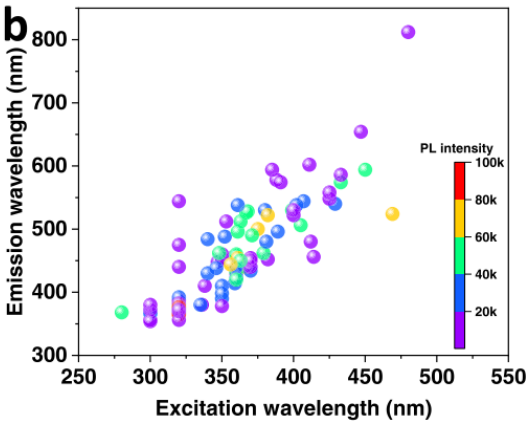
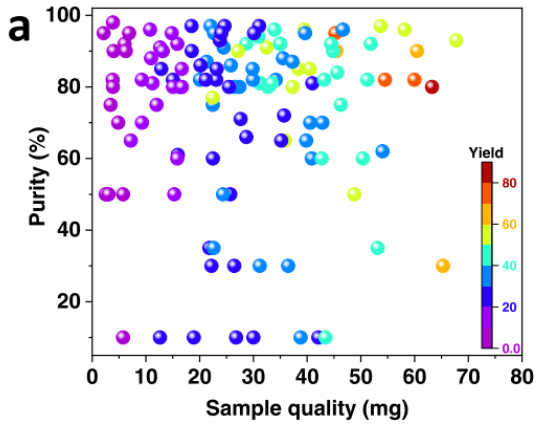
Energy level



Drop casting



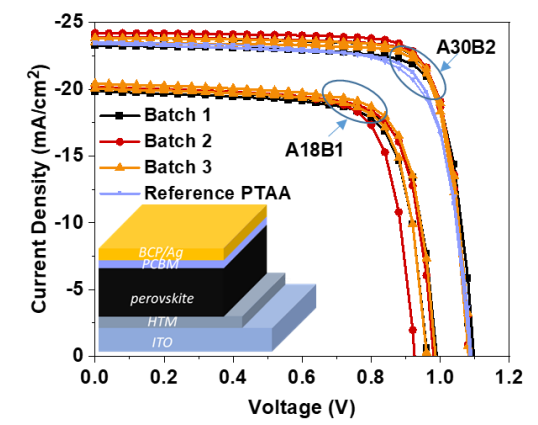
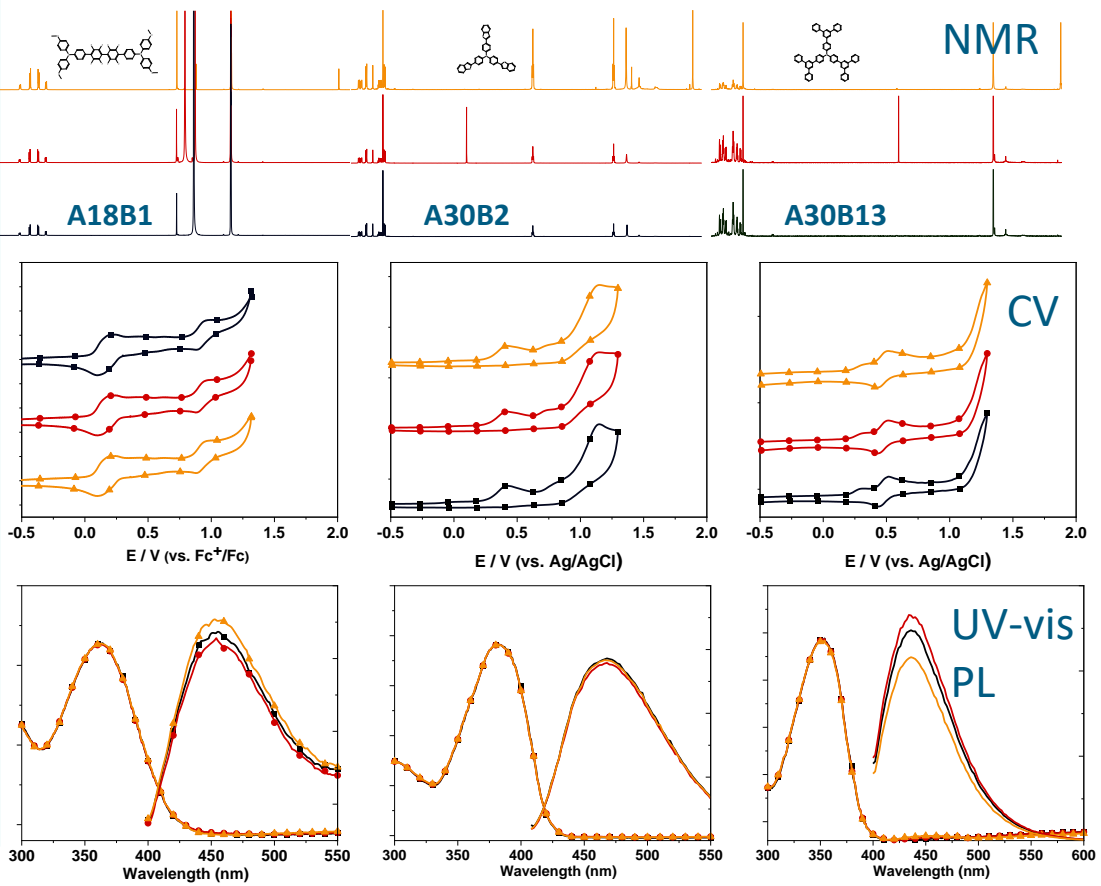
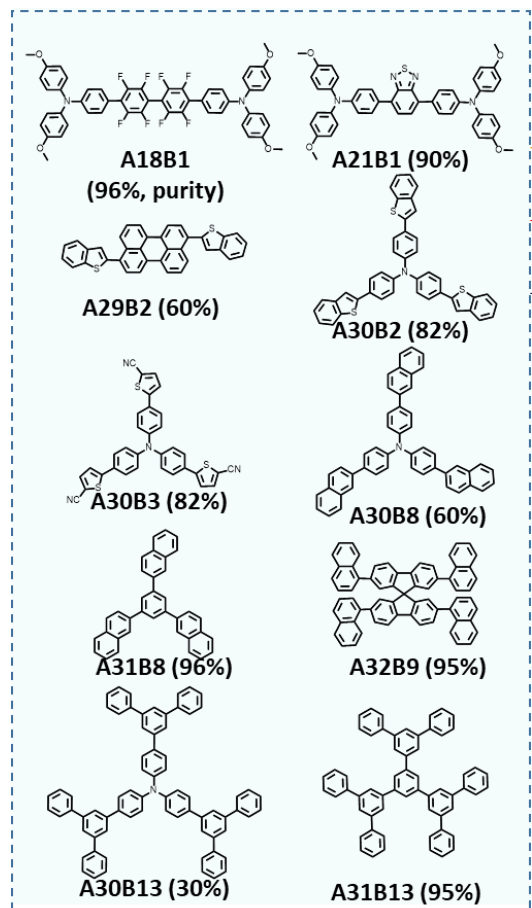
Local electrochemistry



Spin coating

Figure 4. Properties of the synthesized compounds: (a) Sample weight, yield, and purity; (b) UV-vis absorption and PL; and (c) HOMO and LUMO based on DFT calculation.

Batch-to-batch repeatability-UV-vis, CV, UV-vis and PL



- ❑ 10 molecules (5, >90%; 2, 80-90%; 2, 60%; 1, 30%)
- ❑ 3 batches synthesis
- ❑ NMR, CV, UV-vis absorption and PL
- ❑ PSCs device

Excellent repeatability!

Thanks for your attention!

Acknowledgments

