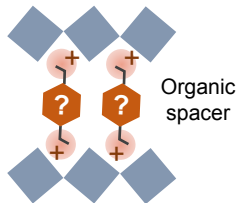


## Existing Compounds

Inorganic Pb-I framework



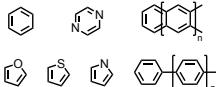
11 experimentally obtained compounds

## Hypothetical Compounds

Organic spacer

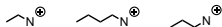
=

$\pi$ -conjugated backbone



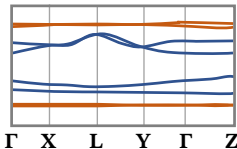
+

Non-conjugated alkyl group

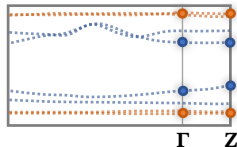


## Electronic Structure

PBE + SOC



HSE06 + SOC



## Quantum Well

Type  $I_a$



Type  $I_b$



Type  $II_a$



Type  $II_b$



DJ perovskite repository

High-throughput DFT calculation

Final candidates