# From the bottom up: Predicting 2D quantum materials to twist and stack

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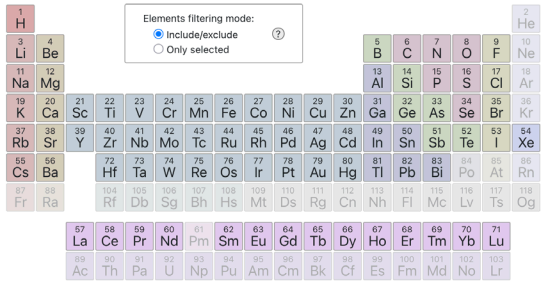
# Materials for correlated phases

RUTGERS–NEW BRUNSWICK
Artificial Intelligence
and Data Science Collaboratory

## Complete database of exfoliable materials



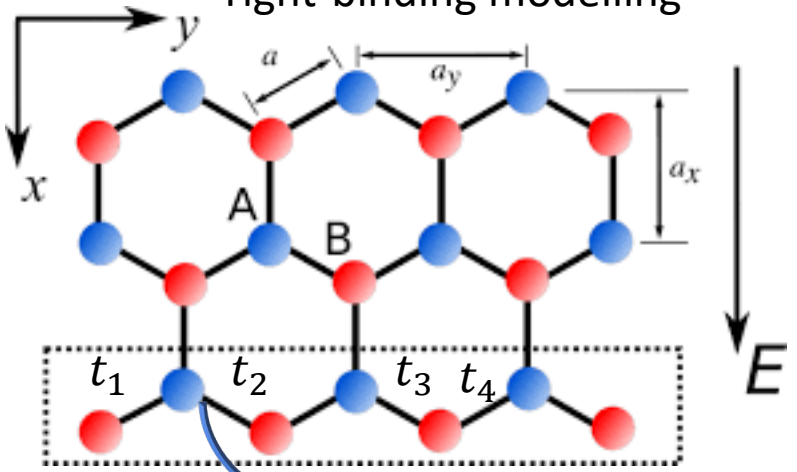

Showing 2702 entries out of 2702

Reset column filters | Show columns

| ID | Formula | Number of elements | Num. of atoms/cell | Space group internationa | Band gap (eV) | Magnetic state | Unstable (soft modes) | Binding energy DF2-CO9 (meV/Å²) | Binding energy rVV10 (meV/Å²) | 3D parent formula |
|---|---|---|---|---|---|---|---|---|---|---|
| mc2d-1 | AgBr | 2 | 4 | $P2_1/m$ | 1.26 | non-magnetic | yes | 7.84 | 14.32 | $Ag_2Br_2O_2Pb_2$ |
| mc2d-2 | $AgClO_4$ | 3 | 6 | P-42m | 2.90 | non-magnetic | no | 19.10 | 28.96 | $AgClO_4$ |
| mc2d-3 | $CuAgTe_2$ | 3 | 4 | Pm | 0.00 | non-magnetic | yes | 24.97 | 29.11 | $AgCuTe_2$ |
| mc2d-4 | $AgF_2$ | 2 | 6 | $P2_1/c$ | 0.00 | non-magnetic | yes | 28.24 | 42.45 | $Ag_4F_8$ |
| mc2d-5 | AgI | 2 | 4 | P4/nmm | 2.15 | non-magnetic | no | 13.50 | 20.78 | $Ag_2I_2$ |
| mc2d-6 | KAgSe | 3 | 6 | P4/nmm | 0.56 | non-magnetic | no | 24.88 | 31.90 | $Ag_2K_2Se_2$ |

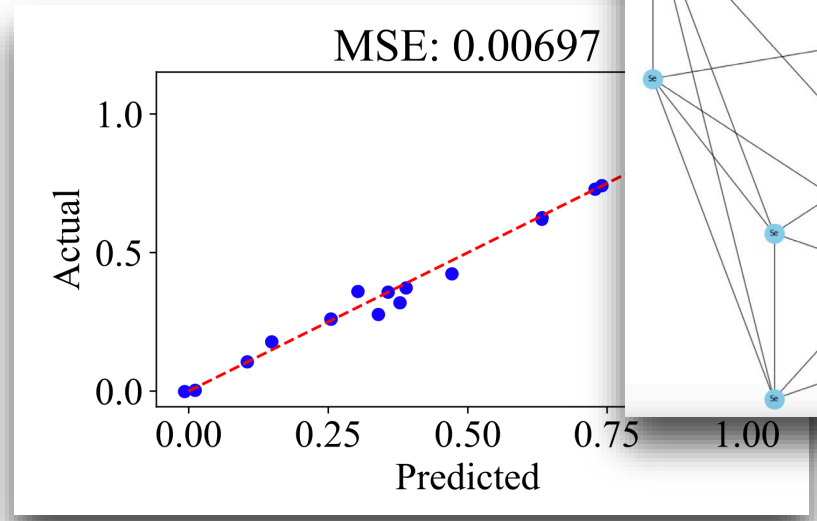
High-throughput DFT

## Tight-binding modelling

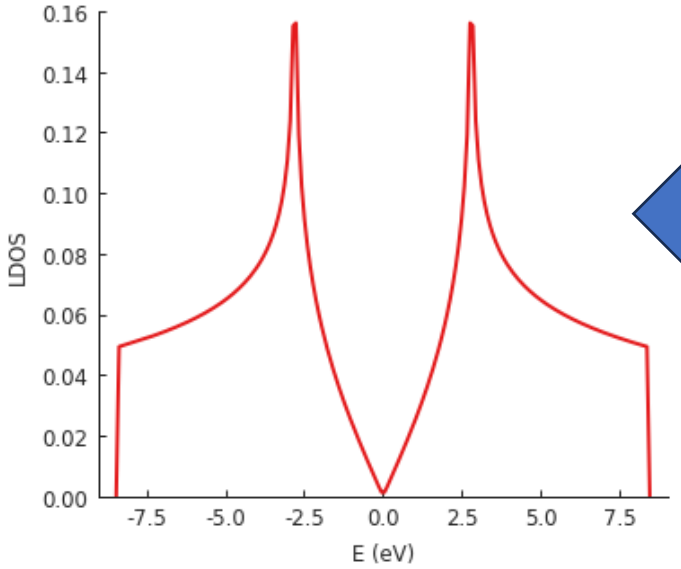



## Tight-binding as a graph

Random forest fitting for long range hopping




(KPM) for local properties



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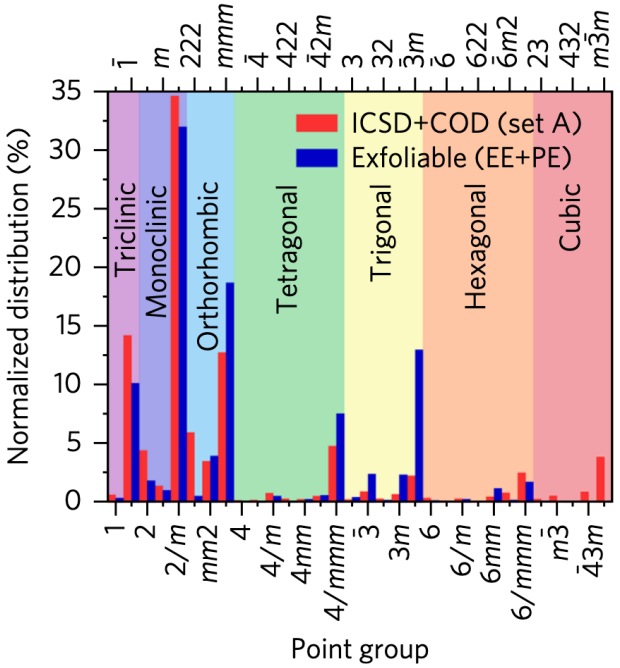
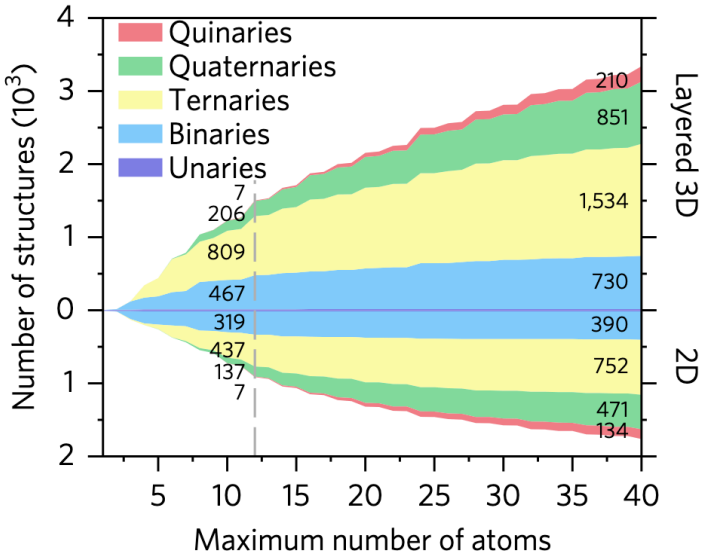
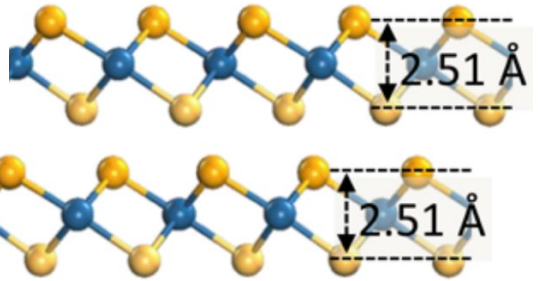
- Material statistics:
  Filter by chemical formula, atomic content, symmetries.

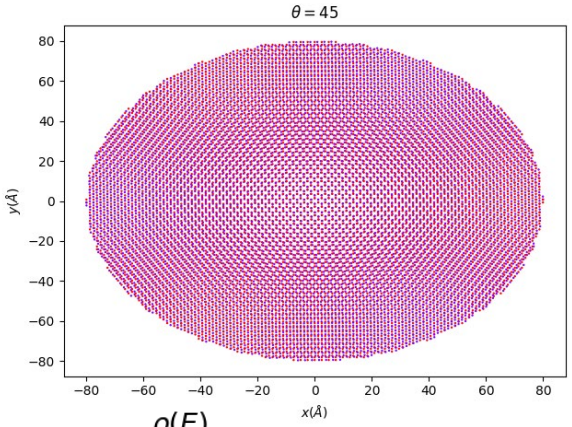


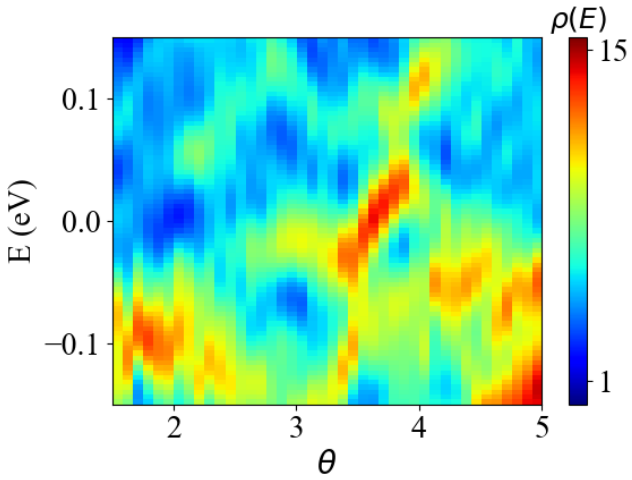




- Identifying a candidate, e.g. $PtSe_2$




DFT + Tight-binding




KPM generated local density
Unit cell ~2000 sites
Computed in minutes
(DFT time: days)