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Semi-empirical modeling of low-dimensional metal-halide perovskites

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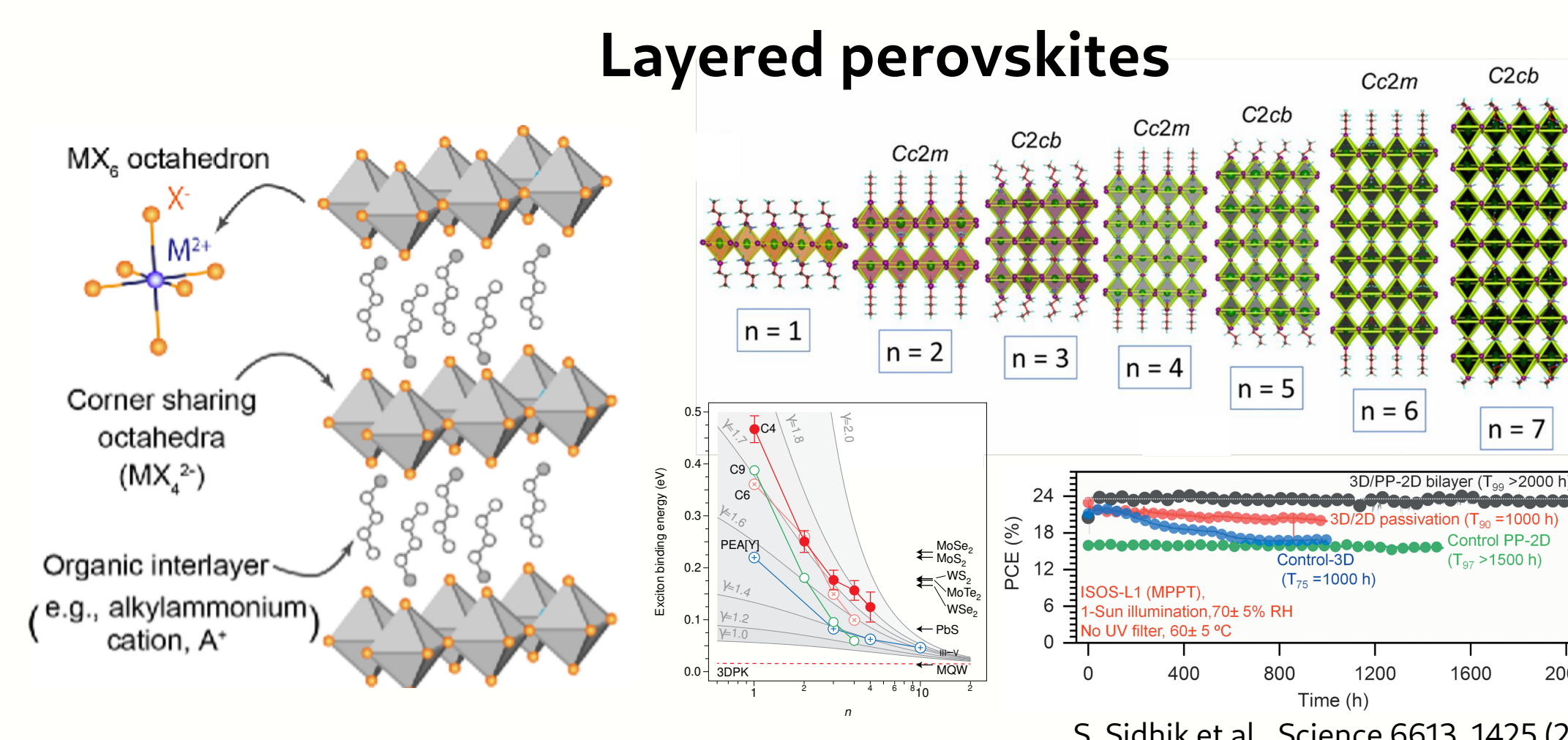
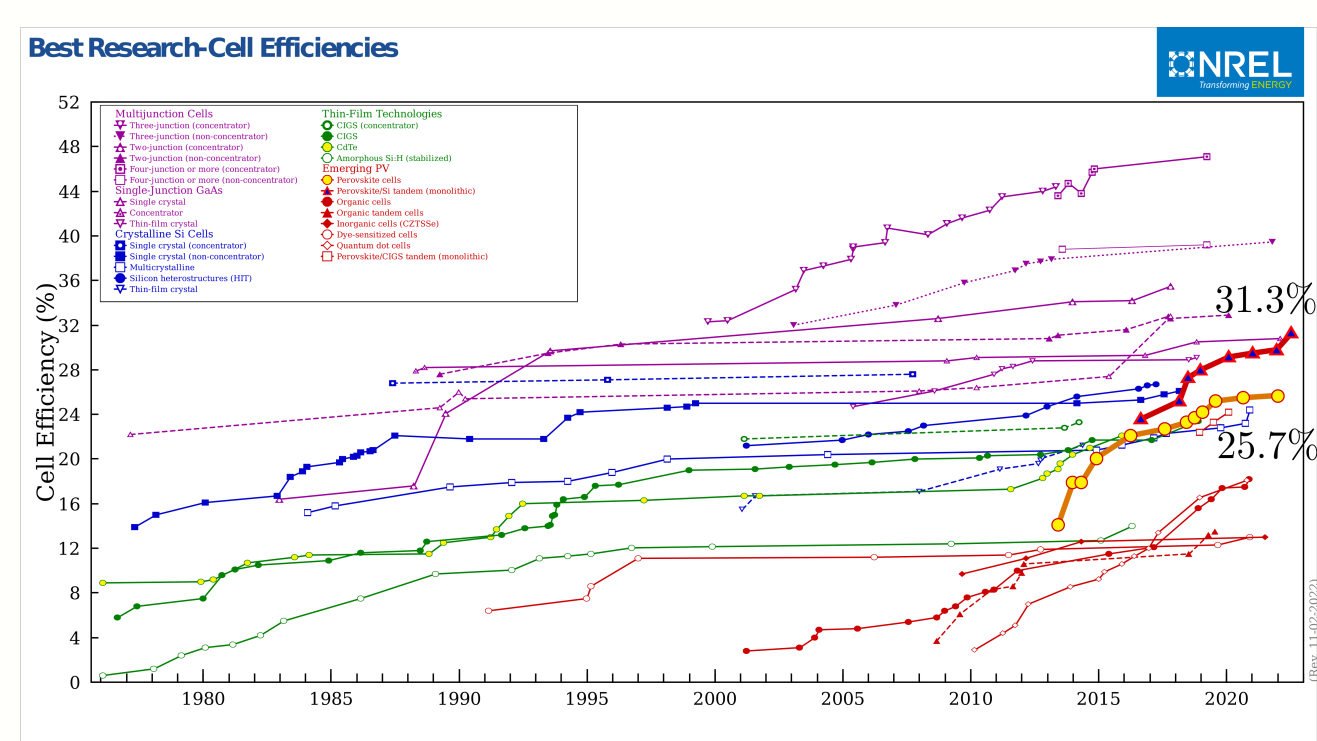
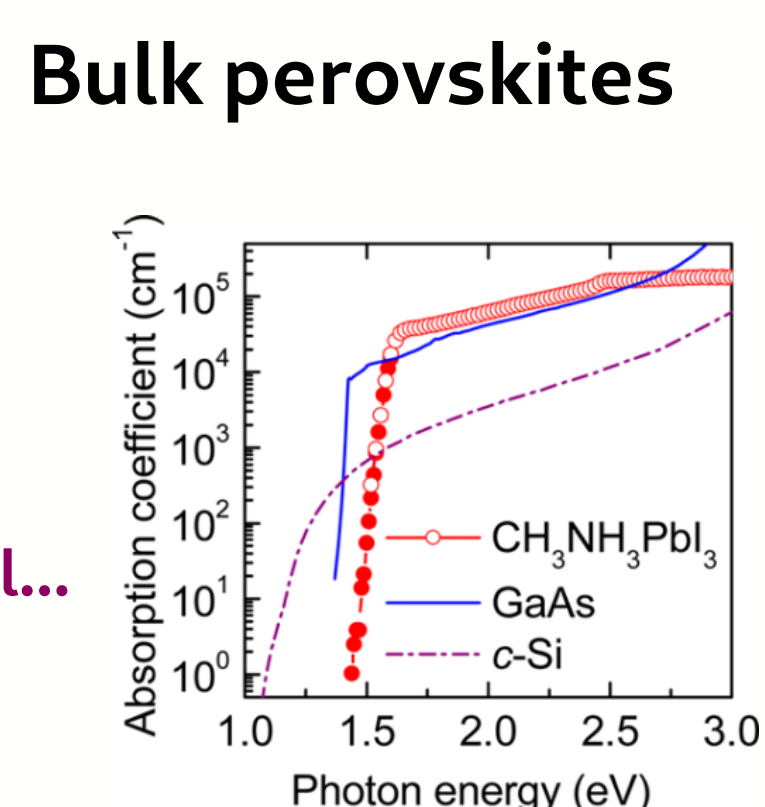
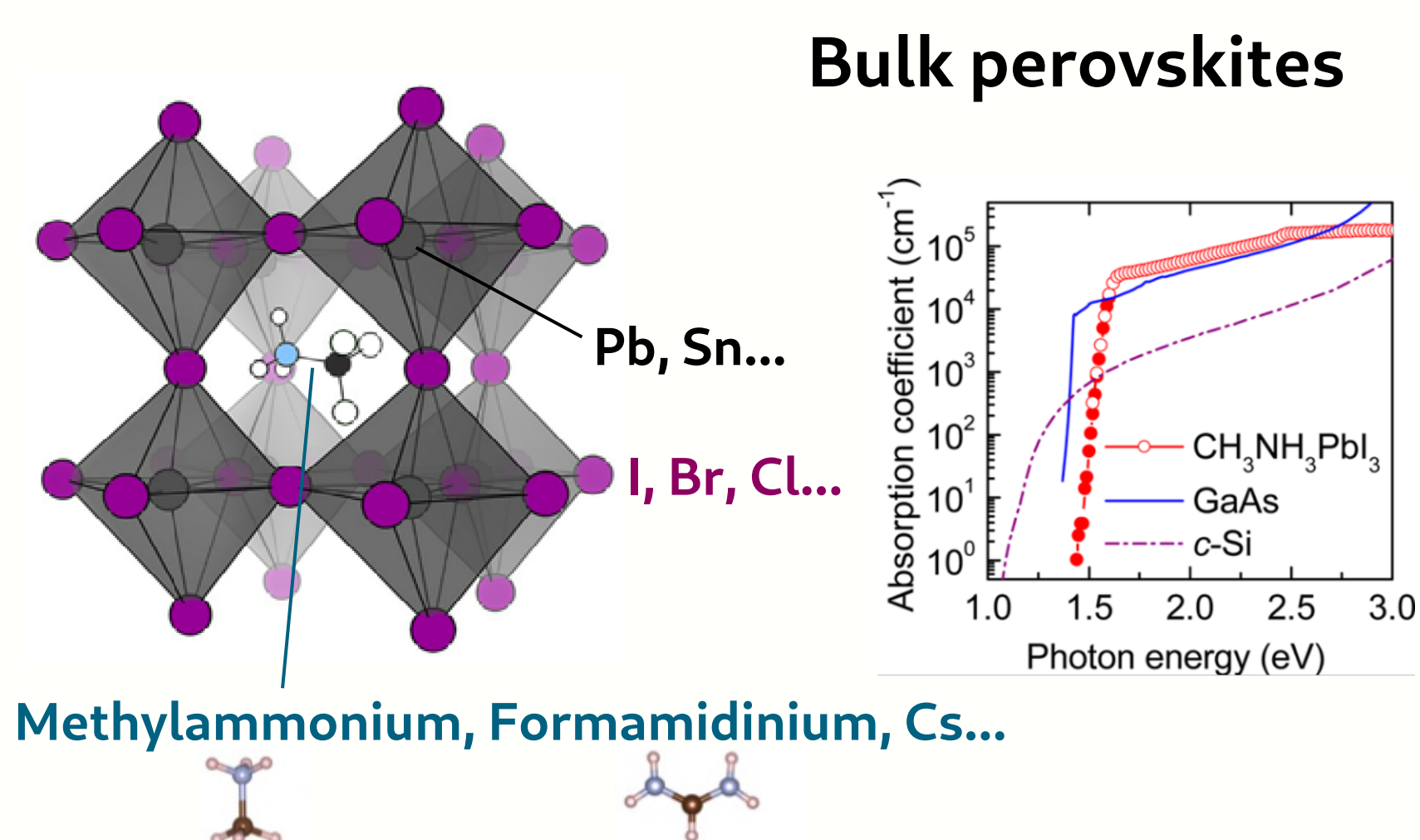
<https://hal.science/hal-04190543v1>

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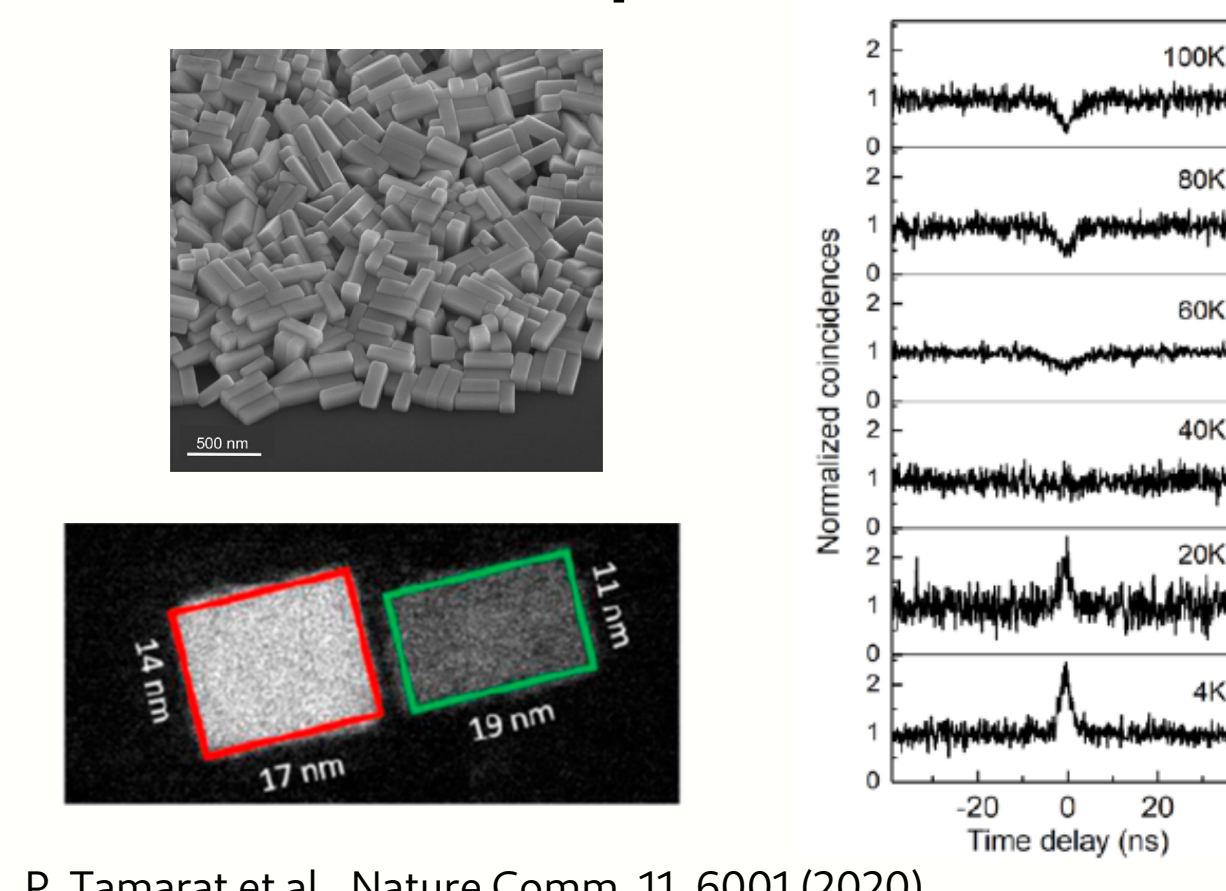
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Metal-halide perovskites as optoelectronic materials



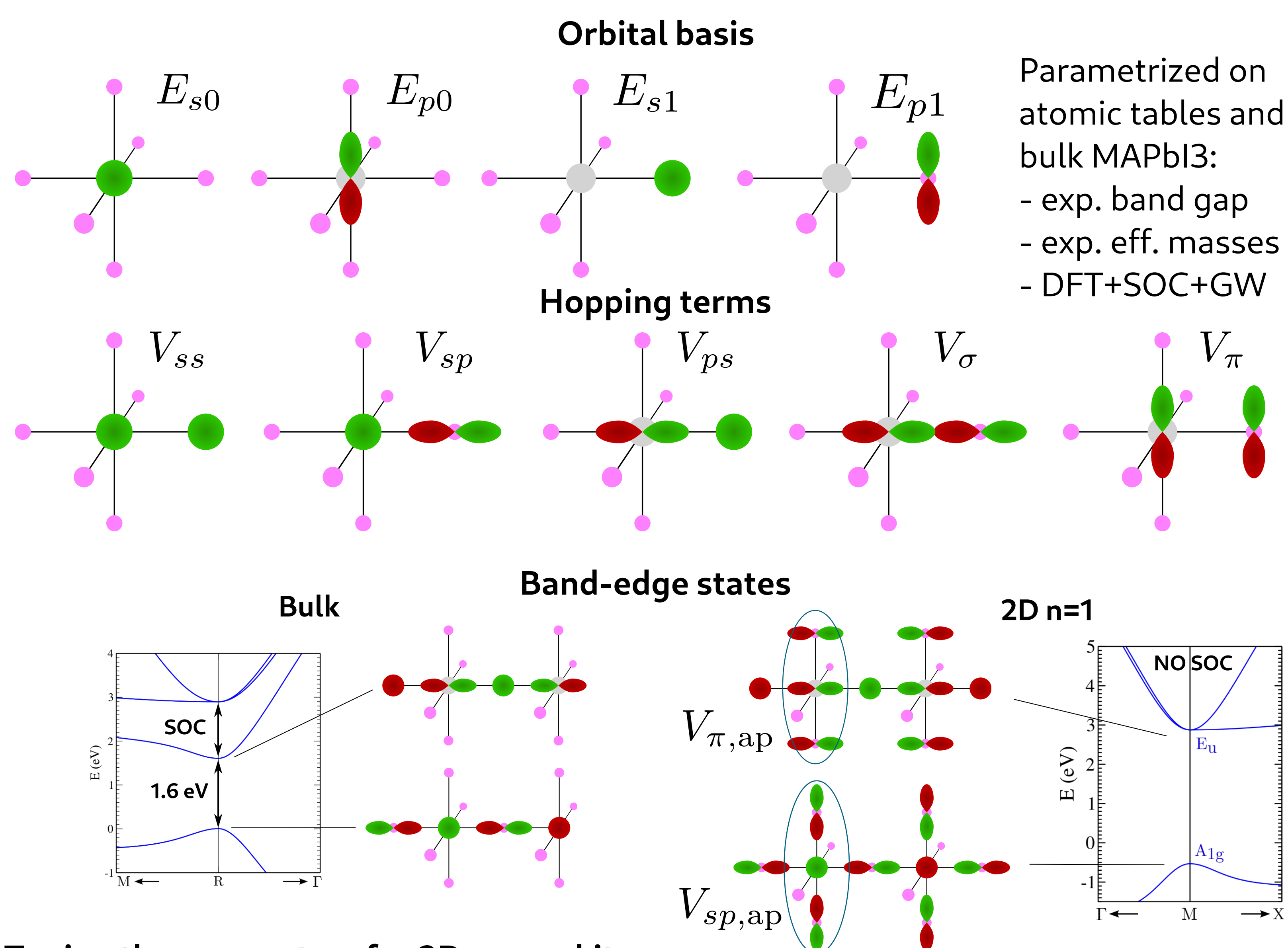
Perovskite quantum dots



S. Sidhik et al., Science 6613, 1425 (2022)

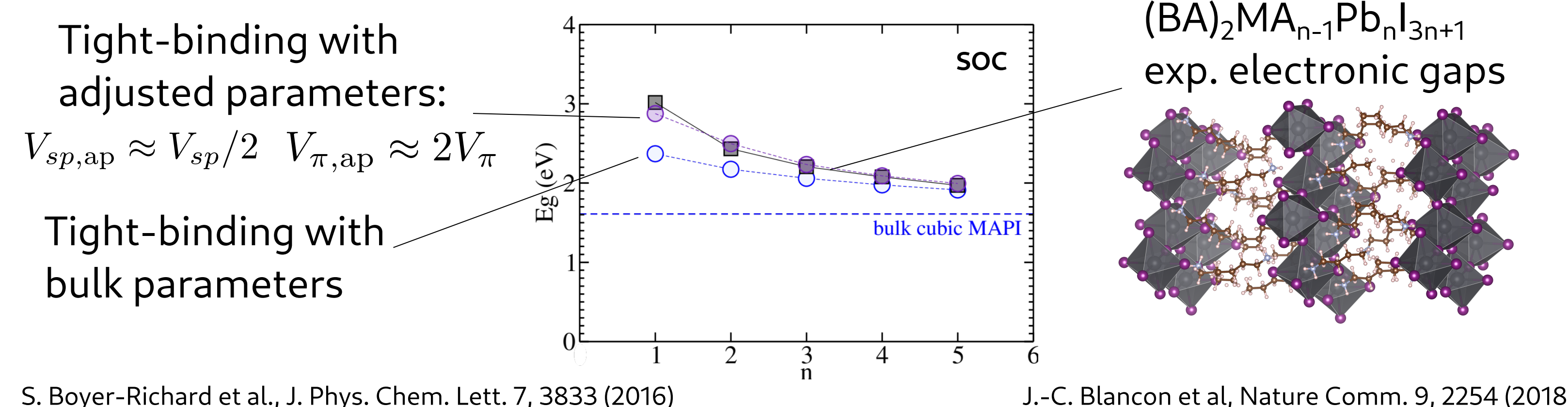
P. Tamarat et al., Nature Comm. 11, 6001 (2020)

Tight-binding modeling of perovskites



Parametrized on atomic tables and bulk MAPbI₃:
- exp. band gap
- exp. eff. masses
- DFT+SOC+GW

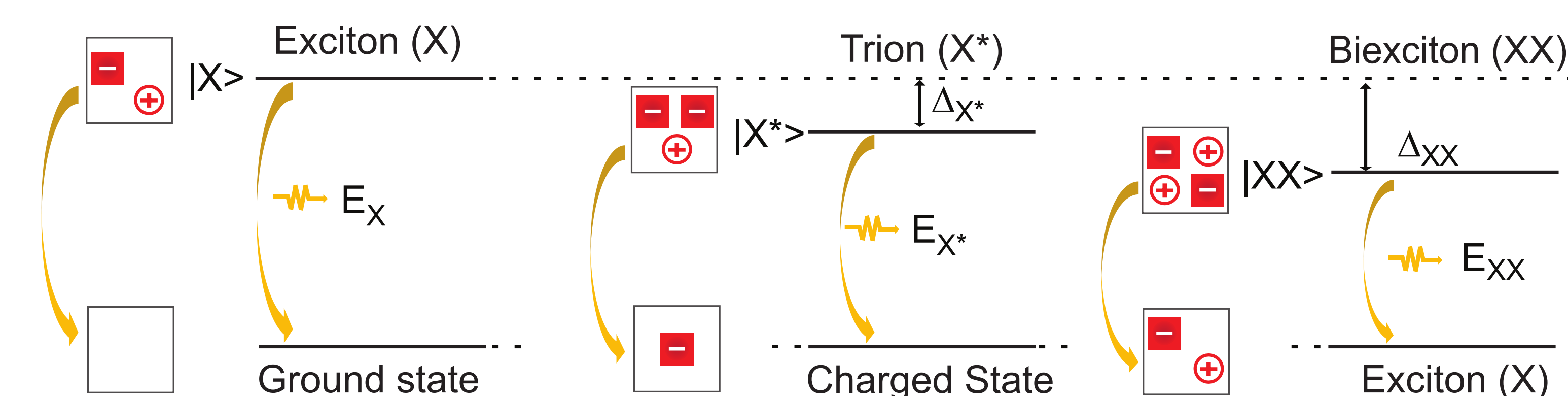
Tuning the parameters for 2D perovskites



S. Boyer-Richard et al., J. Phys. Chem. Lett. 7, 3833 (2016)

J.-C. Blancon et al, Nature Comm. 9, 2254 (2018)

Multiexcitons in perovskite quantum dots



Configuration interaction

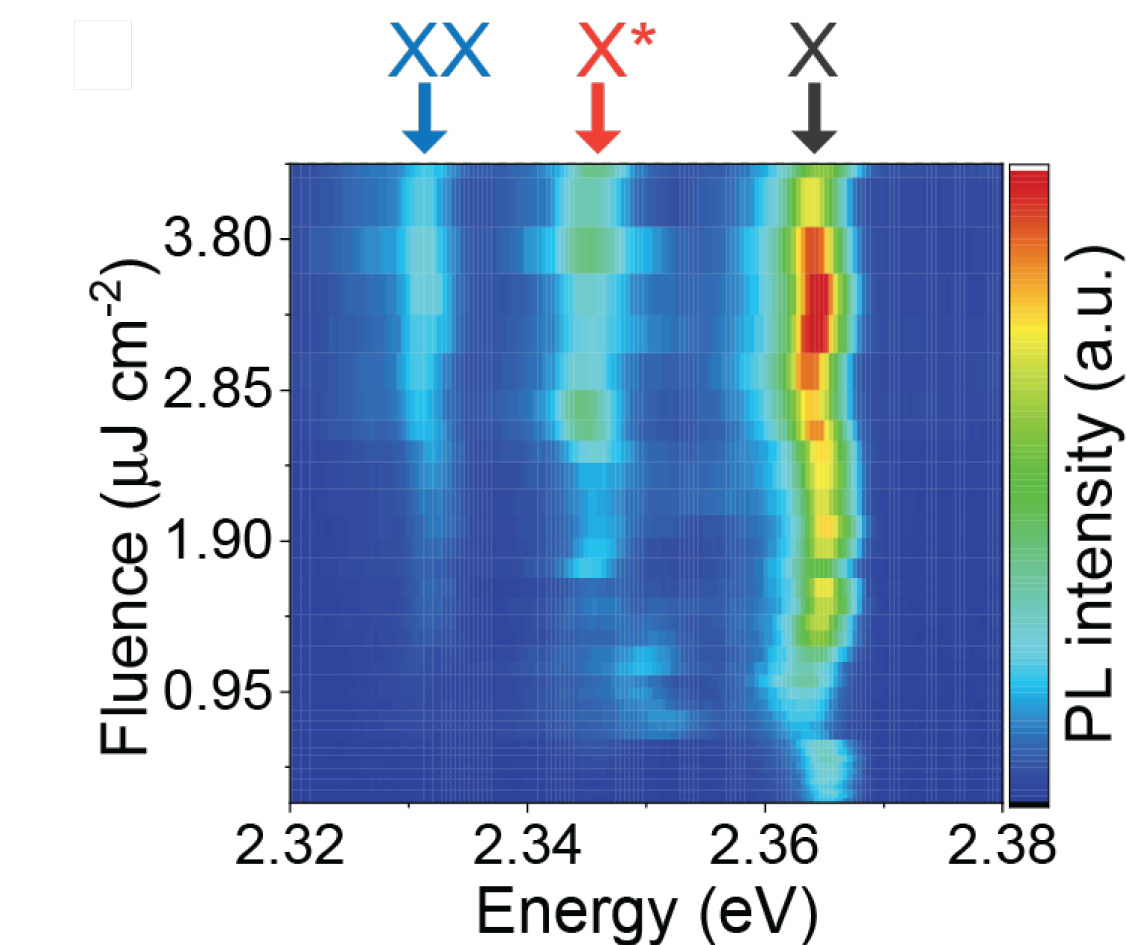
$$\sum_{eh} (H_{eff})_{e'h',eh} A_{eh}^{\alpha} = \omega_{\alpha} A_{e'h'}^{\alpha}$$

Effective mass model:

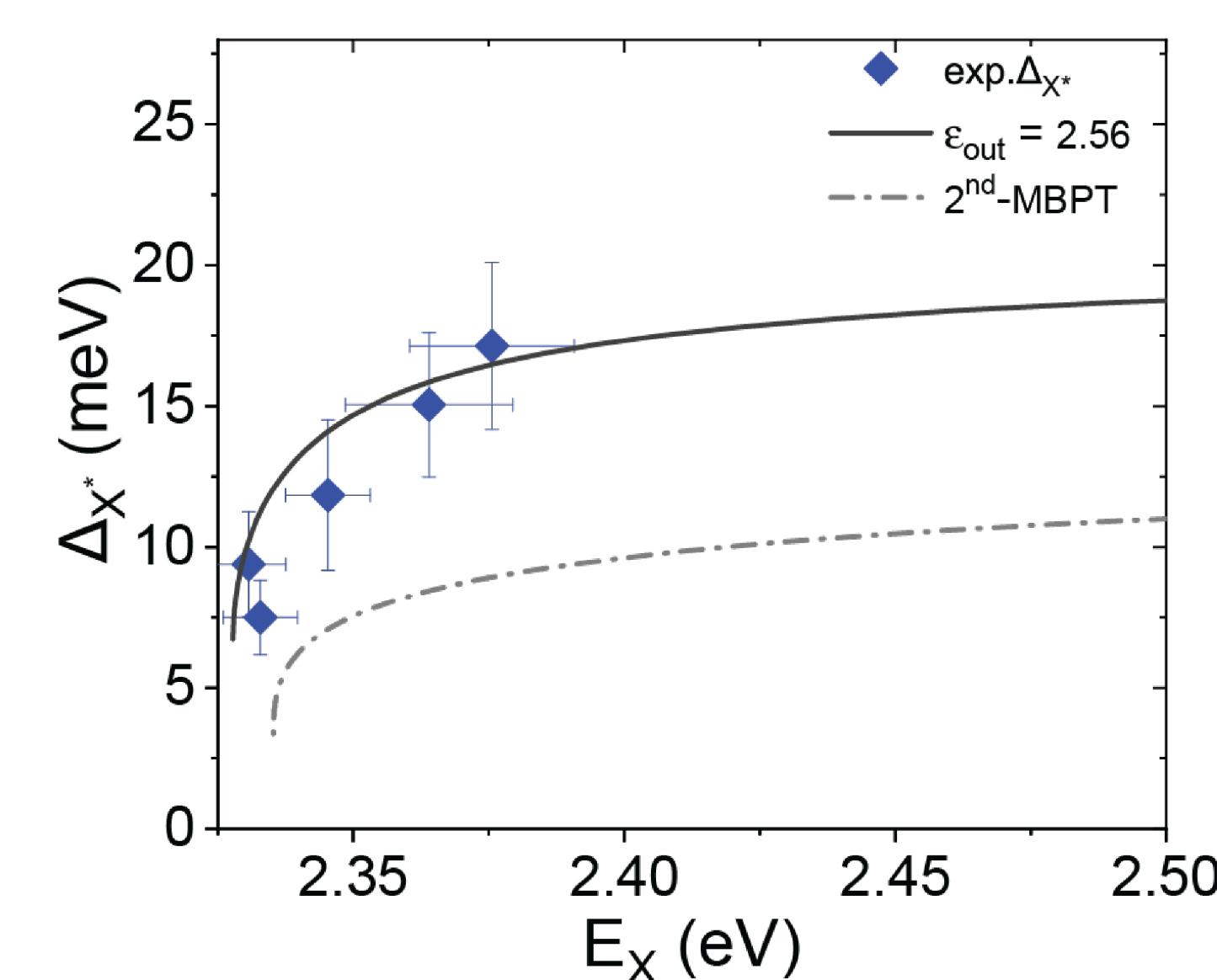
$$(E_e^0 + E_h^0) \delta_{e',e} \delta_{h',h} + V_{e'h',eh}$$

Exciton state: $|\alpha\rangle = \sum_{eh} A_{eh}^{\alpha} |\psi_e\rangle \otimes |\psi_h\rangle$

Photoluminescence measurements



Multiexciton binding energies



Zhu, C. et al., Advanced Materials, 2208354 (2022)

Tamarat, P. et al., Nature Comm. 14 (1), 229 (2023)