DFT bypass with machine learning for the prediction of exciton binding energy in perovskite solar cells

Migon Choi (Duke University)

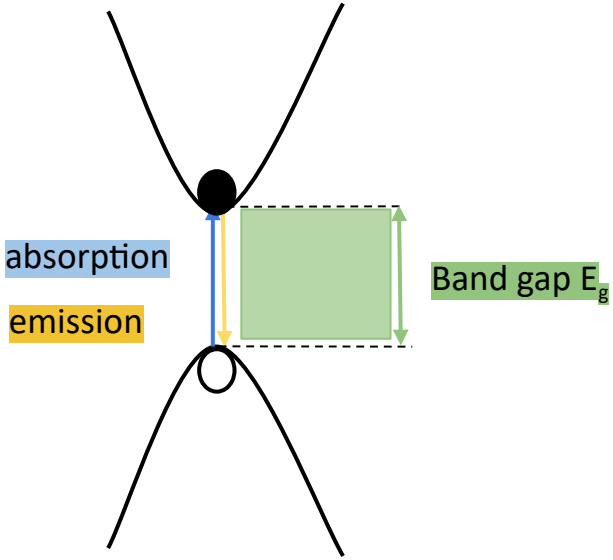
Aaron Peng (University of Chicago)

Cindy Wong (University of Illinois Urbana-Champaign)

Optical properties with and without excitonic effects in direct semiconductors

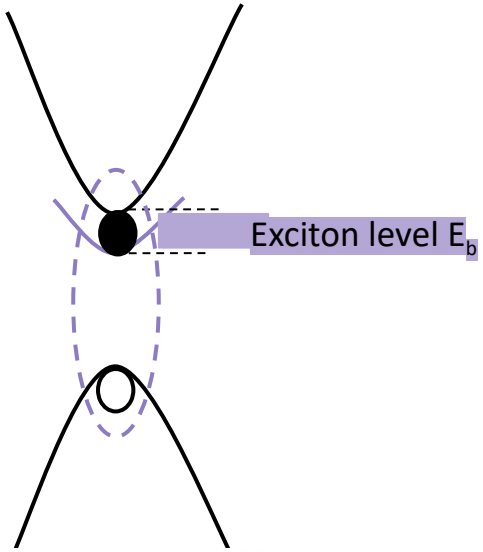
Independent-electron approximation

Conduction band



Valence band

Inclusion of excitonic effects



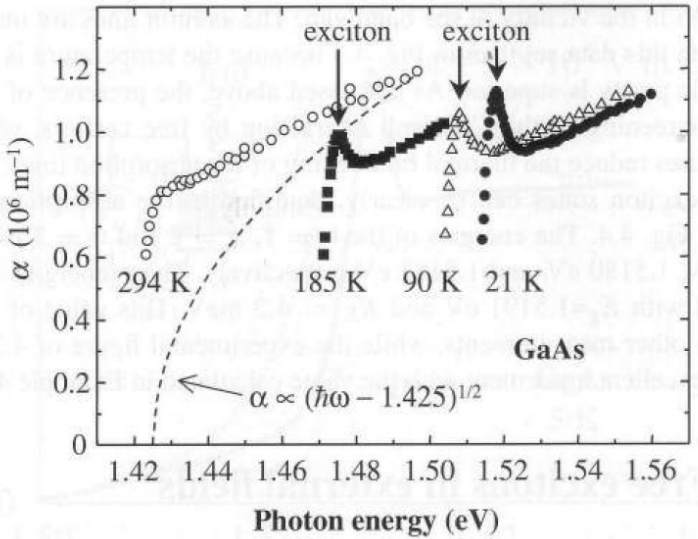
$$E_b = E_g - \frac{R_0 \mu}{n^2 m_0 \epsilon_r^2}$$

R_0 Rydberg constant

μ Reduced effective mass

ϵ_r Dielectric constant/ screening term

Ex: GaAs with and without excitonic effects [1]

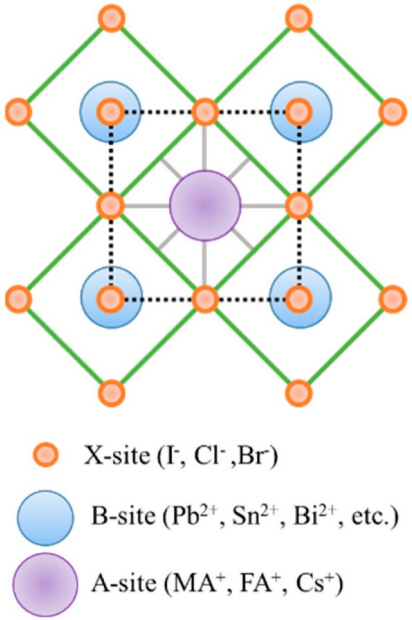


[1] Sturge, M. *Physical Review*, (1962) 127(3), 768.

E_g @ 294K: 1.425eV

Excitons in perovskites

Highly polarizable lattice



Major controversies in calculating exciton binding energy

$$E_b = E_g - \frac{R_0 \mu}{n^2 m_0 \epsilon_r^2}$$

R_0 Rydberg constant
μ Reduced effective mass
ϵ_r Dielectric constant/ screening term

1. Which dielectric constant to use? Static (eps = 5) or high-frequency one (eps = 30)?
2. How to account for change in Eb w.r.t temperature?

Ablation of features in deep NN to obtain most relevant features

NREL Transforming ENERGY

- 34,940 ABX3 materials
- 23 features

OQMD The Open Quantum Materials Database

- 23,112 ABX3 materials
- 7 features

C2DB

- 120 ABX3 materials
- 101 features

descriptors

Band Gap

Formation Energy

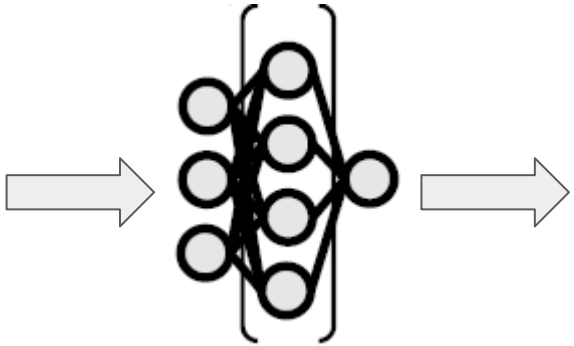
Stability

Ionic radii and atomic volume of abx

Lattice constant

…

Fully connected deep NN



LassoCV as classical ML benchmark

Exciton binding energy