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



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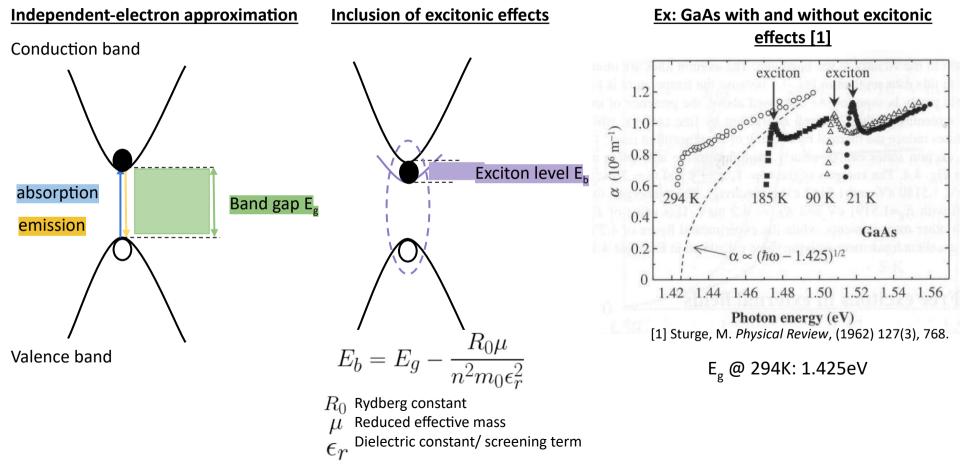


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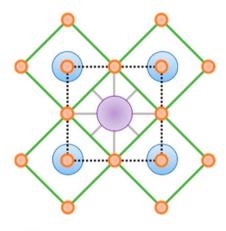


Optical properties with and without excitonic effects in direct semiconductors

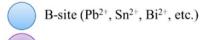


Excitons in perovskites

Highly polarizable lattice



X-site (I⁻, Cl⁻,Br⁻)



A-site (MA⁺, FA⁺, Cs⁺)

Major controversies in calculating exciton binding energy

$$E_b = E_g - \frac{R_0 \mu}{n^2 m_0 \epsilon_r^2} \begin{array}{l} R_0 \text{ Rydberg constant} \\ \mu \text{ Reduced effective mass} \\ \epsilon_r \text{ Dielectric constant/ screening term} \end{array}$$

- Which dielectric constant to use? Static (eps = 5) or highfrequency 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



- 34,940 ABX3 materials
- 23 features



- 23,112 ABX3 materials
- 7 features



- 120 ABX3 materials
- 101 features

descriptors

Band Gap

Formation Energy

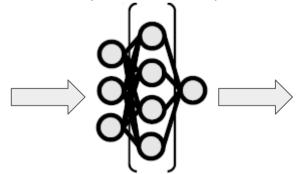
Stability

Ionic radii and atomic volume of abx

Lattice constant

...

Fully connected deep NN



Exciton binding energy

LassoCV as classical ML benchmark