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Enhancing Performance of V_2O_5 Cathodes in Li-ion Batteries through First-Principles-Based Heterostructure Engineering & Controlled Doping

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AIMS Artificial Intelligence & Modeling for Materials Science

Computational Materials Science & Catalysis

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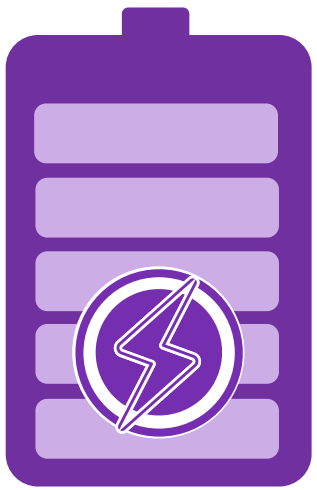
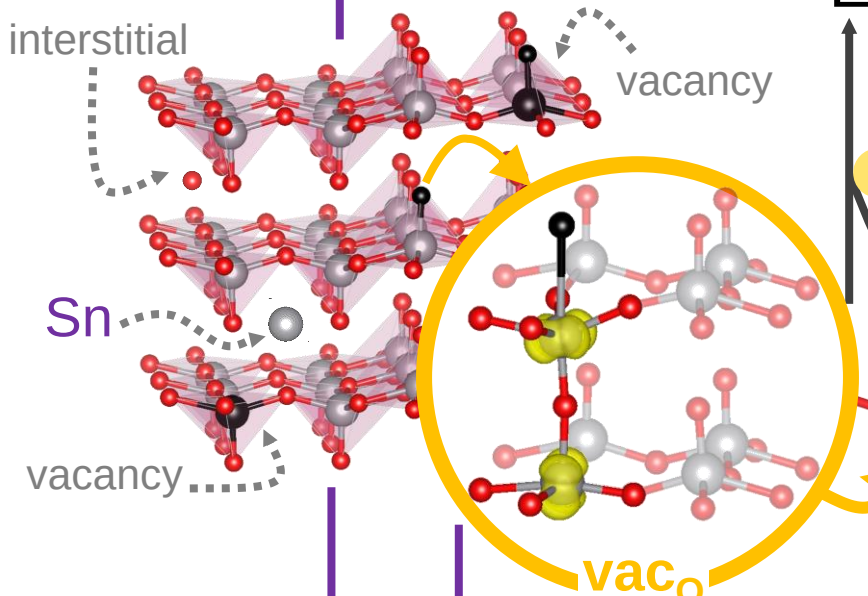
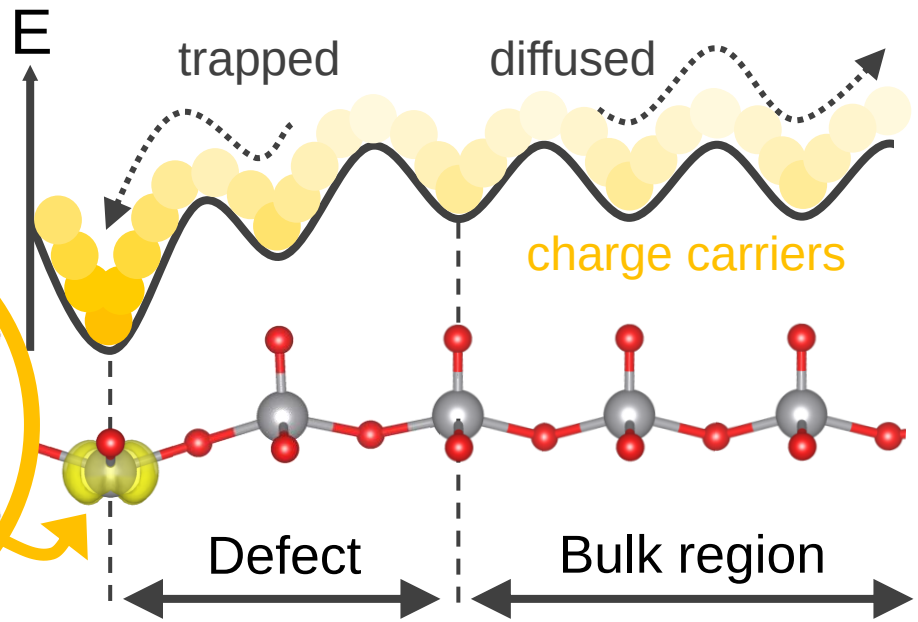
Outlines

Li-ion batteries (LIBs) (overview)

Sn-doped V_2O_5 as a cathode of LIB







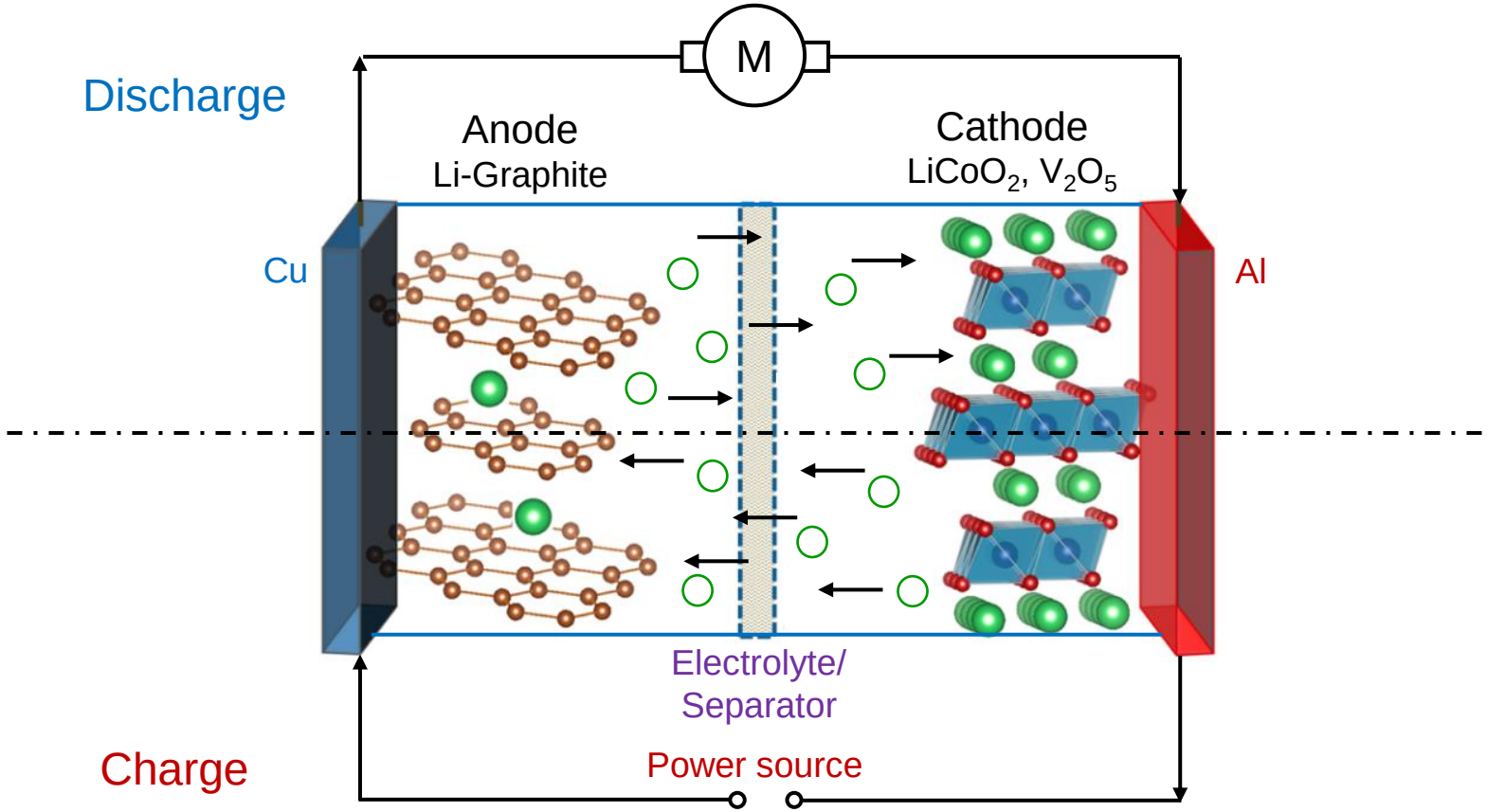
(1) Individual point defect (Sn-doped V_2O_5)

(2) The dominant defect and charge compensation

(3) Charge transport

Role of Sn doping

Li-ion battery: how it works



Electronic and ionic conductivities play an important role on the performance.

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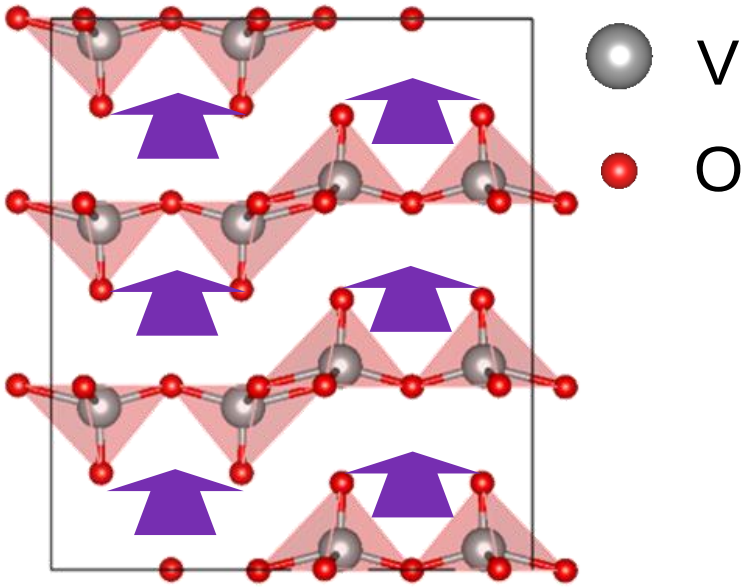
V_2O_5 as cathode material

V_2O_5 → layered structure → accommodate Li^+ → cathode material



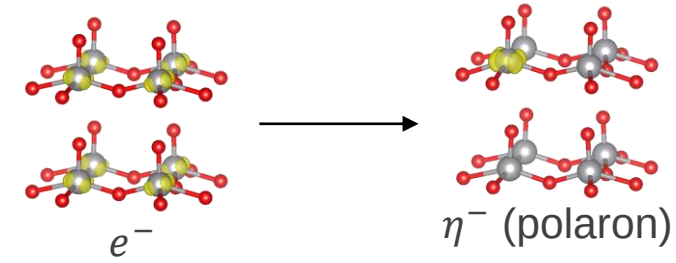
crystal structure of V_2O_5

- high theoretical capacity 442 mAh g^{-1} (commercial $LiCoO_2$: 272 mAh g^{-1})
- inexpensive

- experimental capacity being far from theory
- poor structural stability
- sluggish electrochemical performance (electronic and Li conductivity)

Electron transport in pristine V_2O_5

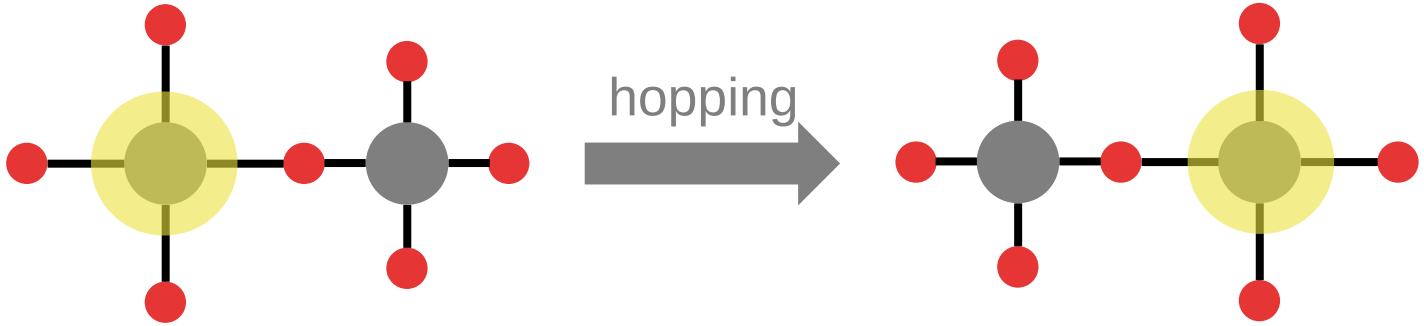
Electron polaron formation

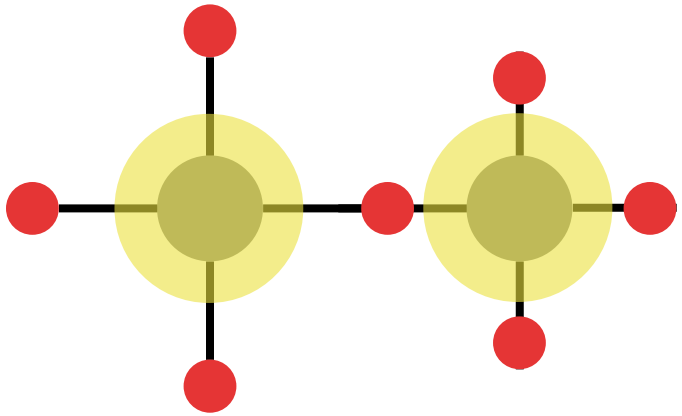


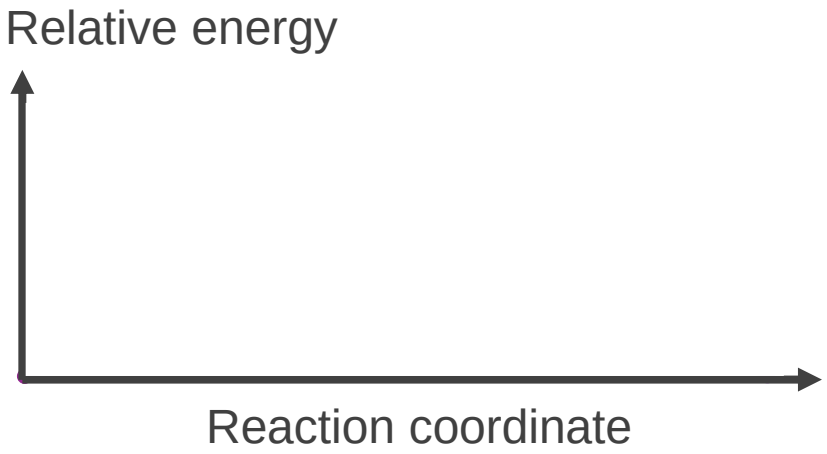
E_{pol} = -0.28 eV

Polaron transport (cartoon)

Top view



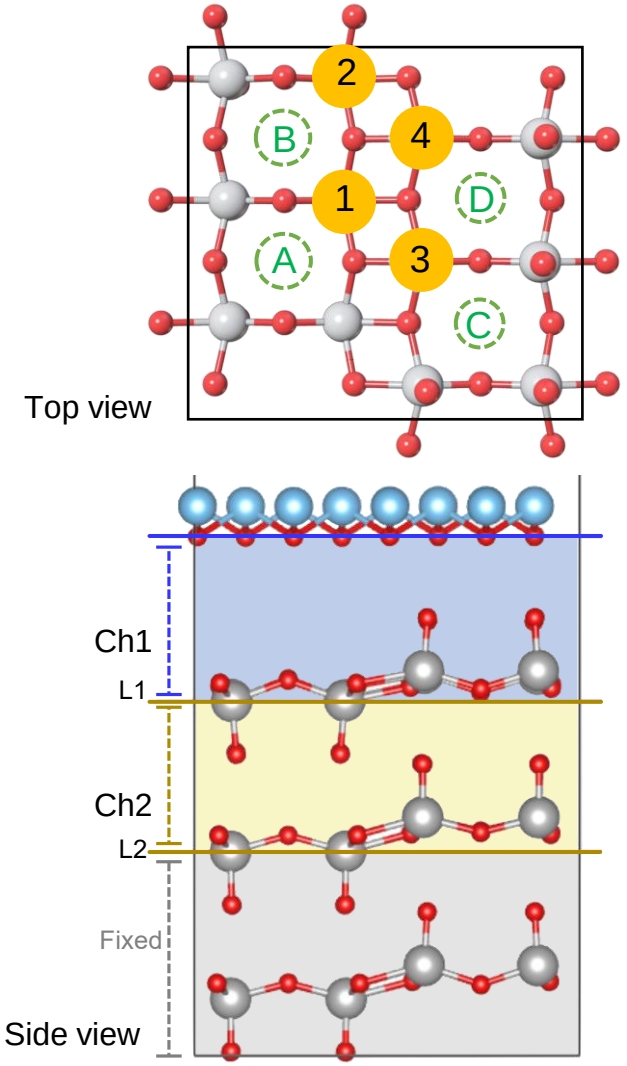


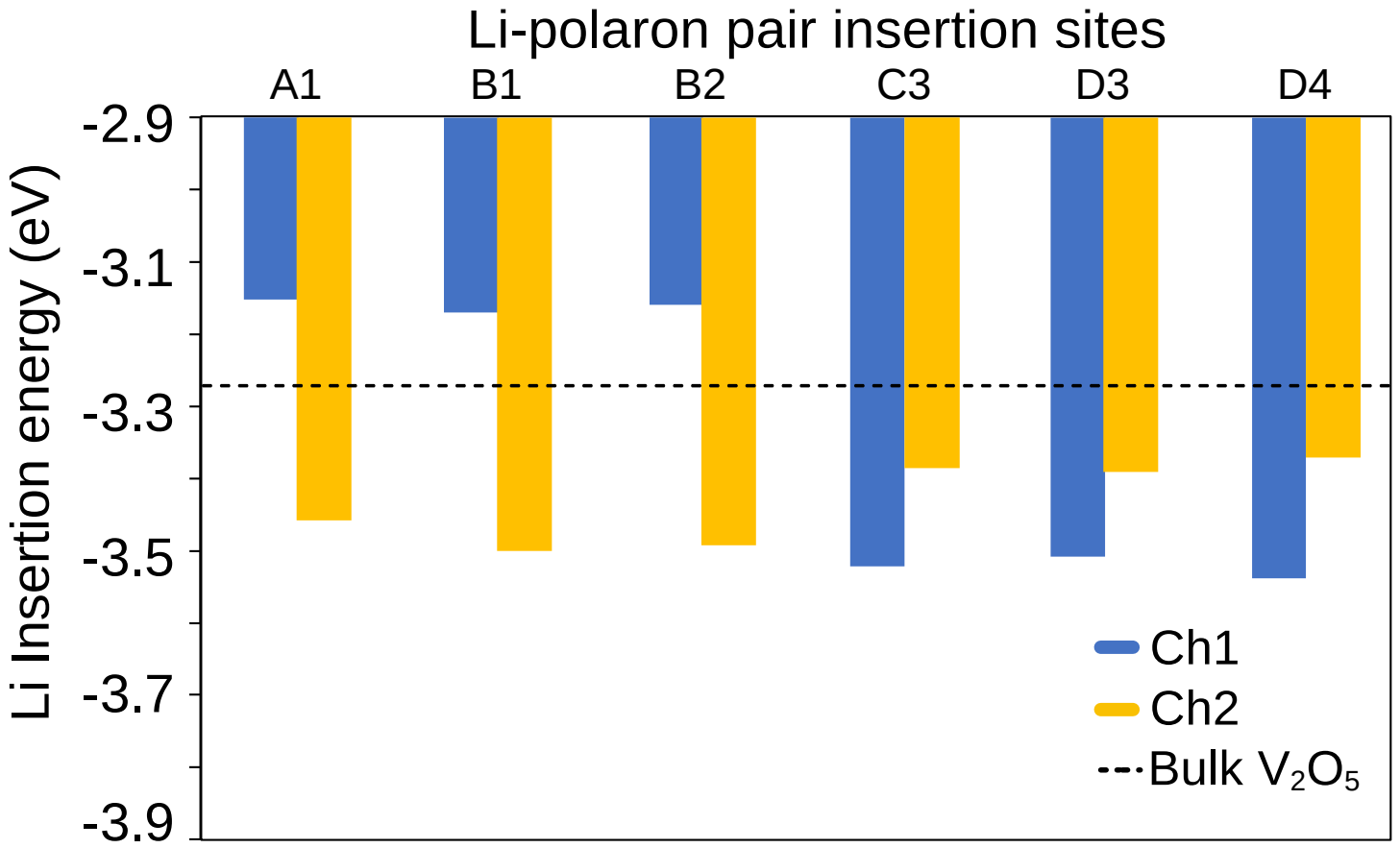


Polaron is preferable to transport in-plane of V_2O_5 with E_a~0.21 eV.

Li insertion

Possible insertion site





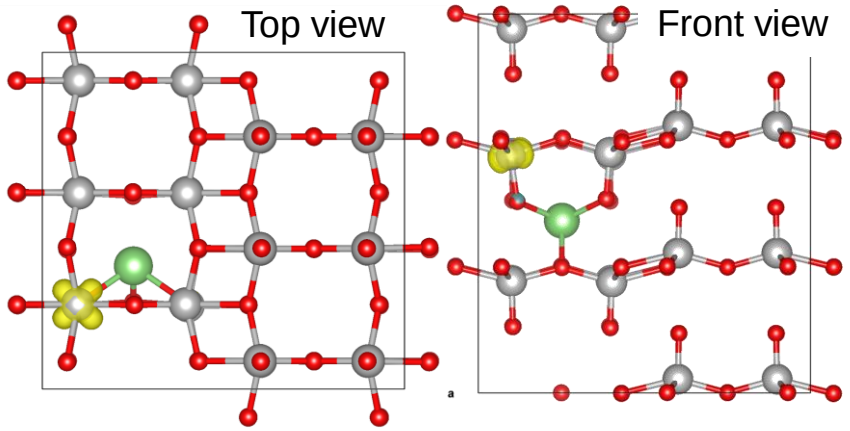
- Heterostructure improves stability of Li insertion

Li intercalation in pristine V_2O_5

Li insertion

Li → Li^+ + polaron

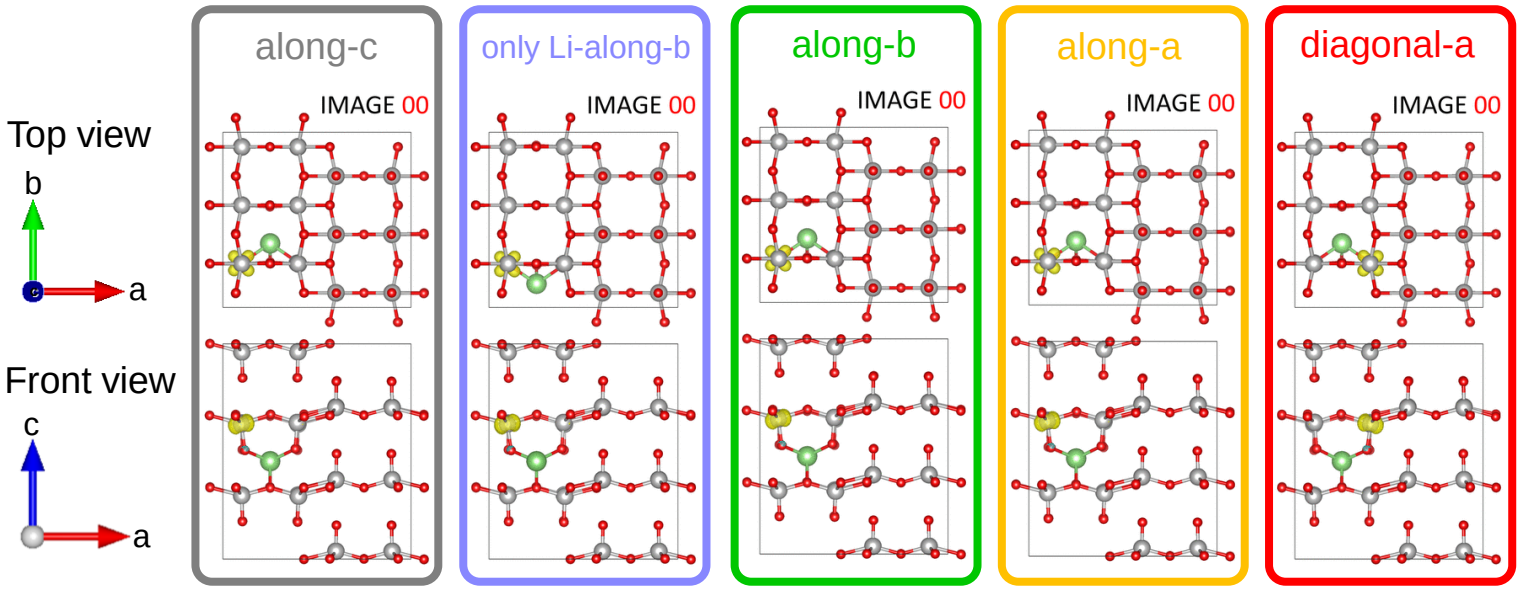
E_{ins} = -3.27 eV



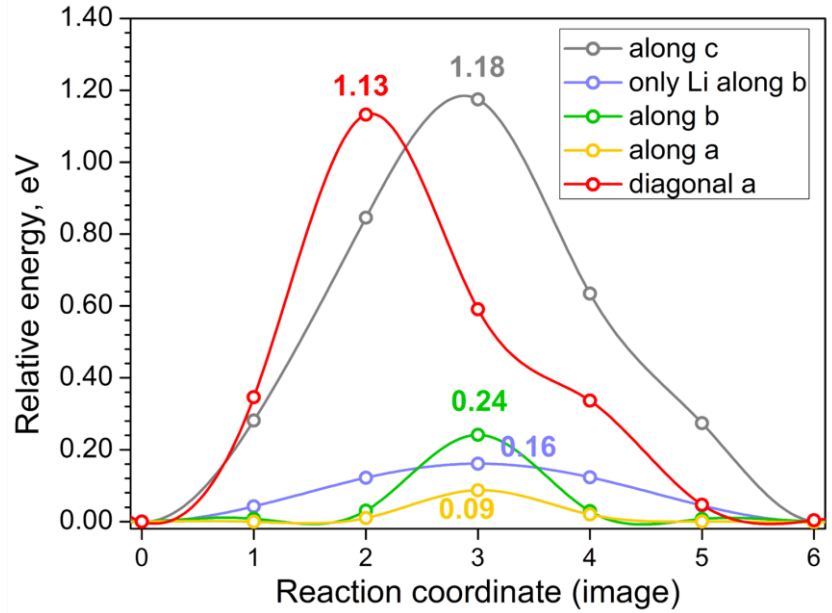
Li diffusion

Li^+ and polaron will migrate in a couple fashion.

Li diffusion pathways



Diffusion barriers

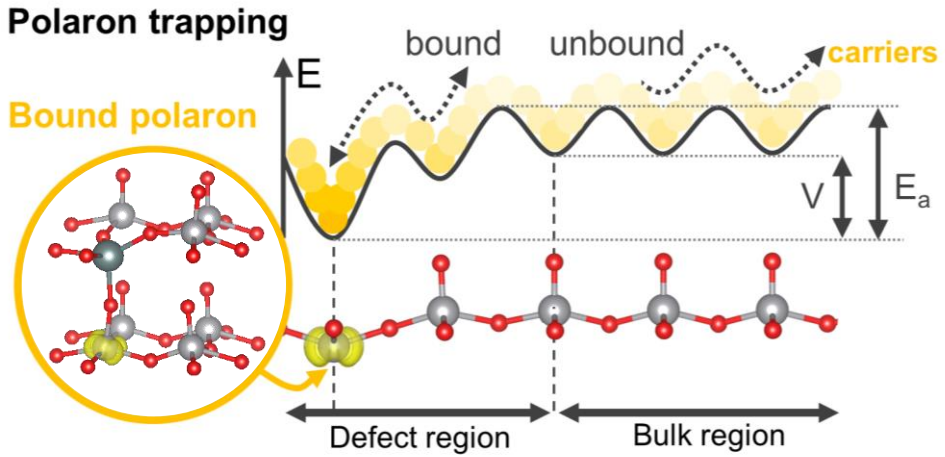


effective diffusion path → along b-direction

Conclusions

- Based on DFEs and concentrations under constraint of charge neutrality, (i) Sn doping increase the concentrations of bound polarons in term of neutral Sn_{VO}.

System	Defect	C_0 (cm^{-3})	V (eV)	E_a (eV)
perfect	-	$4x10^4$	0.00	0.21
without Sn	vac_{O1}	$3x10^{16}$	0.41	0.61
with 1%Sn	Sn_{VO}	$1x10^{20}$	0.37	0.56



- These polarons are confined in the thermodynamic potential well (V). However, they can hop away from the defect region by overcoming the effective barrier (E_a), becoming unbound polarons (carriers).
- (ii) Sn doping decrease the interaction between bound polarons and defect center (lowering V and E_a).
- As a result, Sn doping plays a significant role in the increase of charge carrier concentration and the electronic conductivity of the material.

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