DFT-calculations for LiB as SEI and anode material $Li_3V_2O_5$: structure and properties

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Outline

1. LiB:

DFT-NEB simulation of Li diffusion in LiB solid electrolyte and calculation of the migration barrier

- Optimization of structure (cell parameters)
- Supercell creation
- NEB calculation

2. $Li_3V_2O_5$

DFT-modeling of Li^+-intercalation in the $Li_3V_2O_5$ anode material

- CIF-creation from literature data and optimization
- Calculation of Li insertion
- Intercalation potentials & volume change calculations

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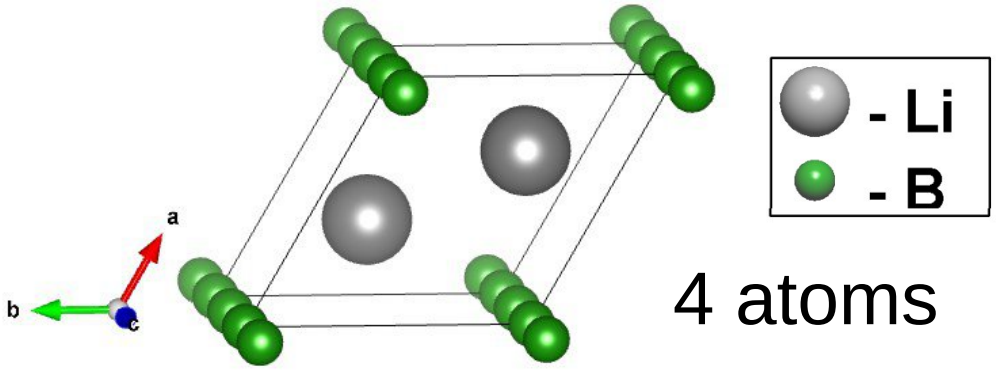
Simulation of Li diffusion in LiB

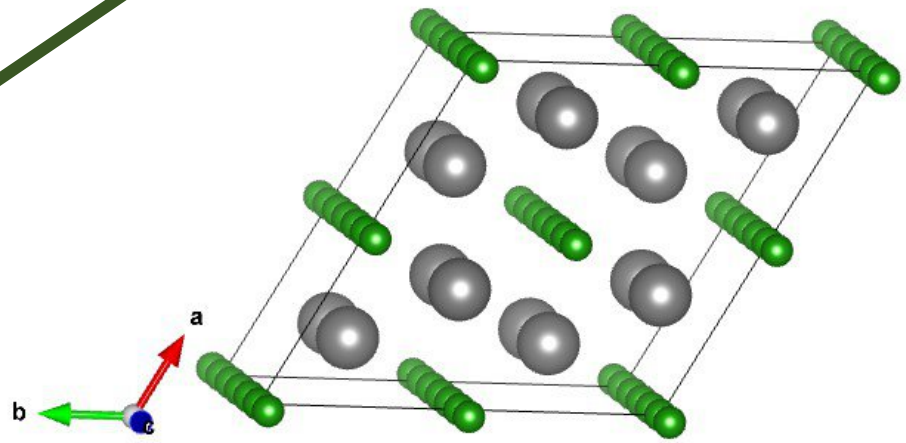
Optimization &Supercell creation

Structure	V, Å³	a, Å	c, Å ɣ=120º
Initial	43.448	4.013	3.115
Optimized	43.482	4.01	3.12



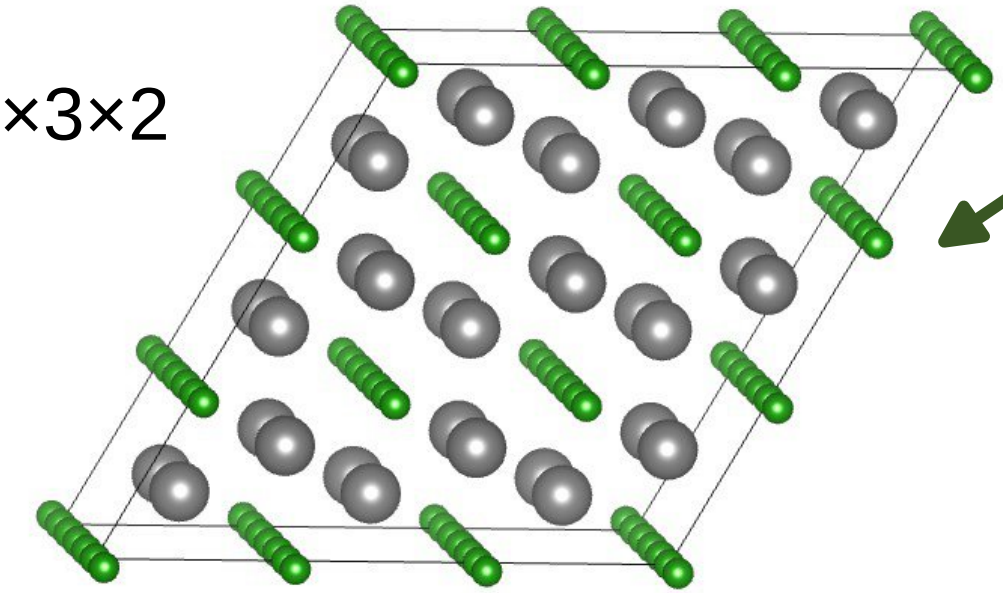
4 atoms

2×2×2



32 atoms

3×3×2



72 atoms

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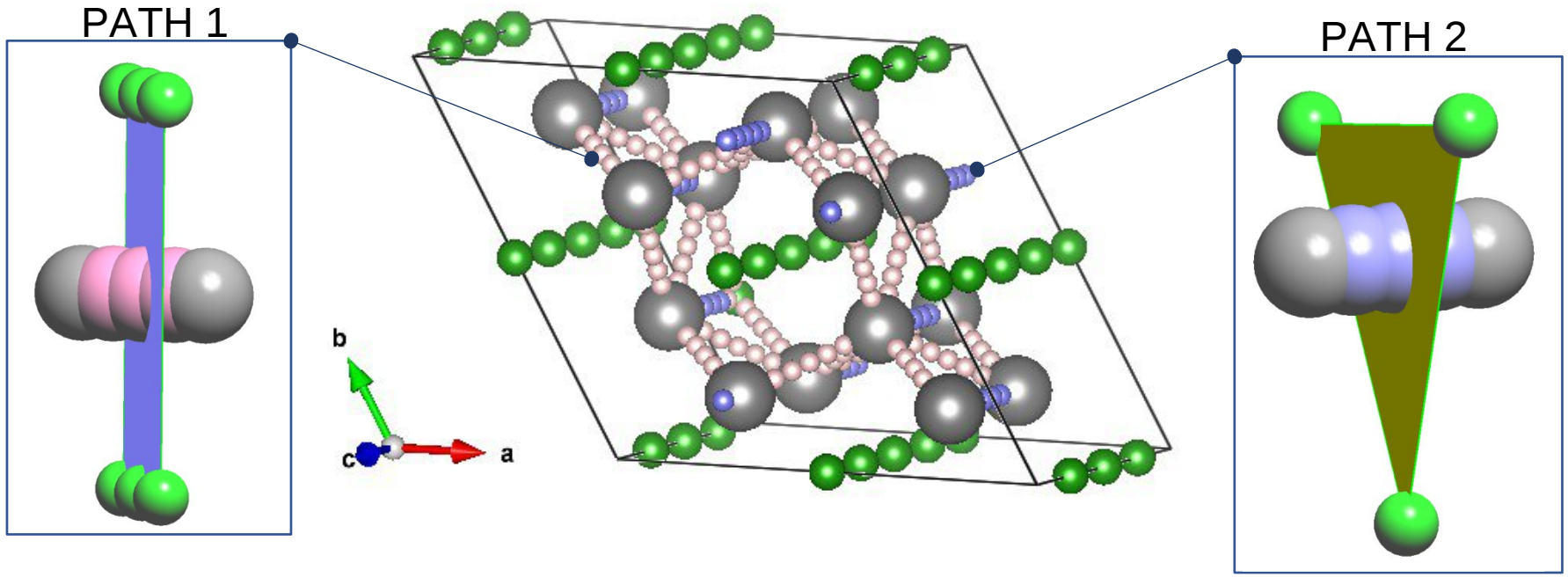
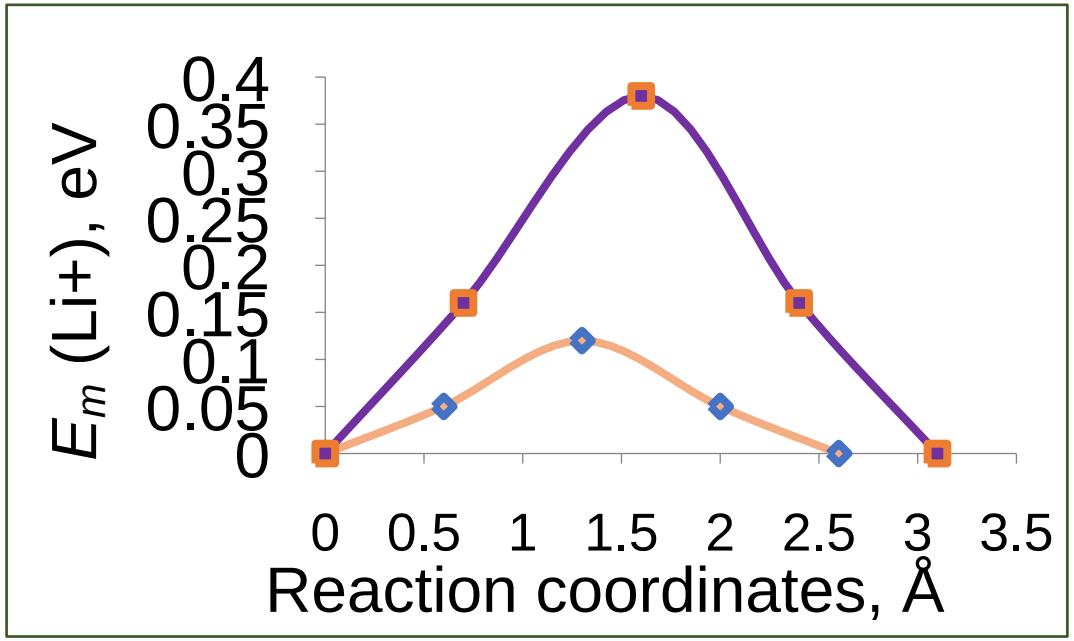
Simulation of Li^+ diffusion in LiB. NEB-calculation





Supercell	E_m (PATH 1), eV	E_m (PATH 2), eV	Calculation time, hour
2x2x2	0.12	0.38	~1
3x3x2	0.17	0.37	~6.5

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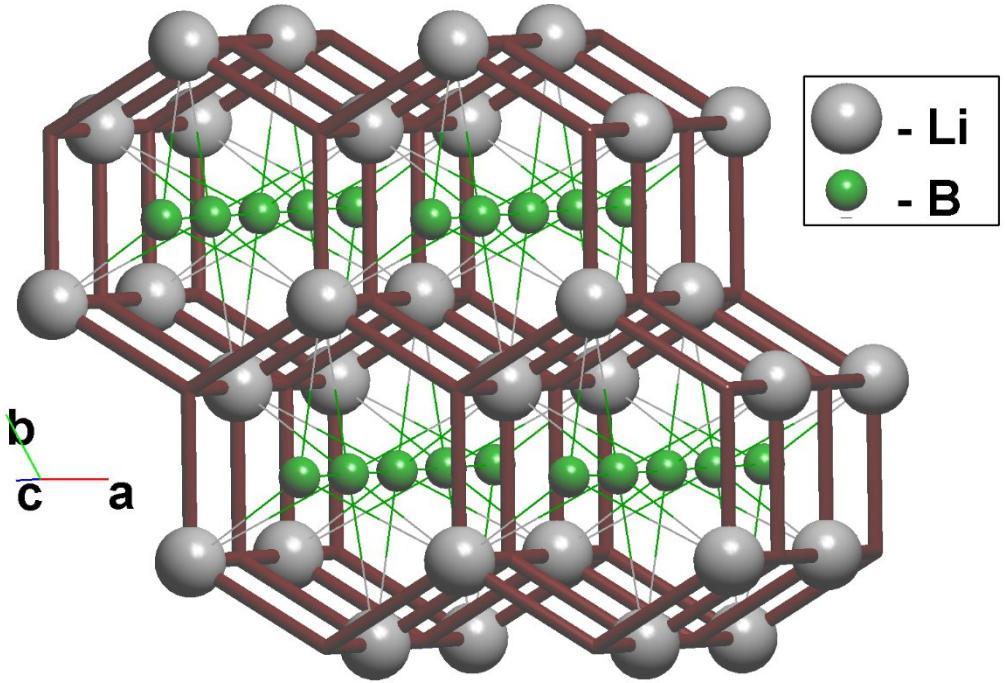
Simulation of Li^+-ion diffusion in LiB. VP & BVS methods

3D Li^+-ion migration map (brown lines) in crystallochemical and BVS methods



E_m (Li^+) = 0.06 eV

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DFT-modeling of Li^+-intercalation in $Li_3V_2O_5$ anode material

nature › articles › article

Article | Published: 02 September 2020

A disordered rock salt anode for fast-charging lithium-ion batteries

Haodong Liu, Zhuoying Zhu, [...] Ping Liu

Nature **585**, 63–67 (2020) | Cite this article

24k Accesses | **79** Citations | **191** Altmetric | Metrics

DRS-$Li_3V_2O_5$, Space Group: $Fm\bar{3}m$

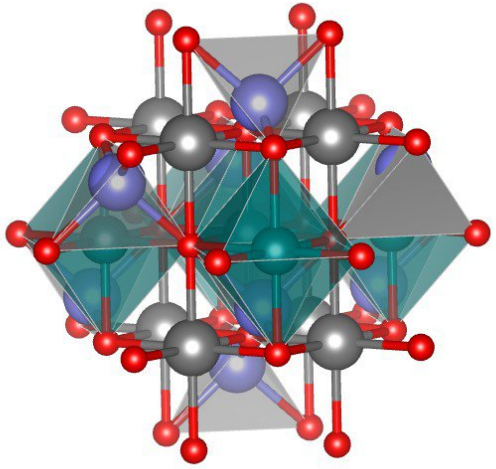
a=b=c 4.095(1) Å,

Neutron pattern: R_{wp}= 2.76%

X-ray pattern: R_{wp}= 2.37%

Atom type	*WyckSymb*	*x*	*y*	*z*	*Occupancy*
Li	4b	0	0	0.5	0.52(1)
V	4b	0	0	0.5	0.4
O	4a	0	0	0	1
Li	8c	0.25	0. 25	0.25	0.04(1)

[redacted] → [redacted] → [redacted] +2 Li →



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DFT-modeling of Li^+ intercalation in $Li_3V_2O_5$ anode material

Compound	V, Å³	a, Å
Initial $Li_3V_2O_5$	68.77(1)	4.097(1)
Optimized $Li_3V_2O_5$	65.548	4.03
Initial $Li_5V_2O_5$	72.56(9)	4.171(3)
Optimized Li5V2O5	85.559	4.41

$$V = -\frac{E(Li_{x_1}V_2O_5) - E(Li_{x_2}V_2O_5) - (x_1 - x_2)E(Li)}{(x_1 - x_2)e}$$

$Li_5V_2O_5$: Li-Li = 1.7 Å

LiCoO2: Li-Li = 2.9 Å

$r(Li_{tetra})$ = 0.59 Å
$r(Li_{oct})$ = 0.76 Å

Used pseudopotential	Intercalation potential, V	Volume increase
PBE	-2.16	32%
PBE-U	-0.88	31%
PBE-U + magnetic	**0.22**	**35%**
Experimental data	0.6	1.8%

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thx.

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