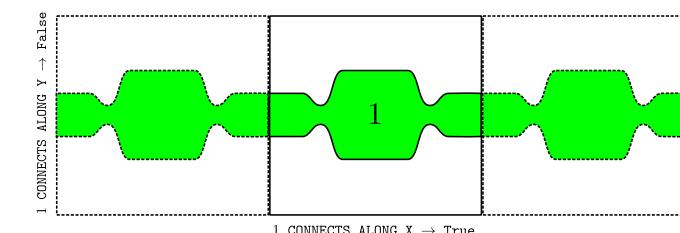
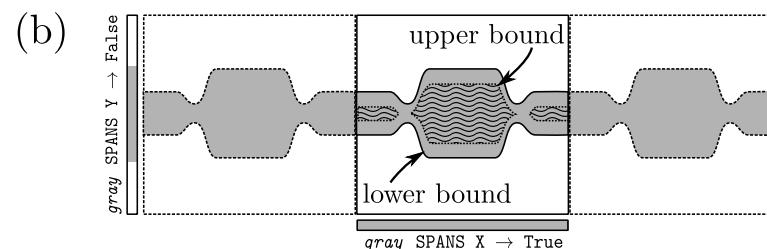
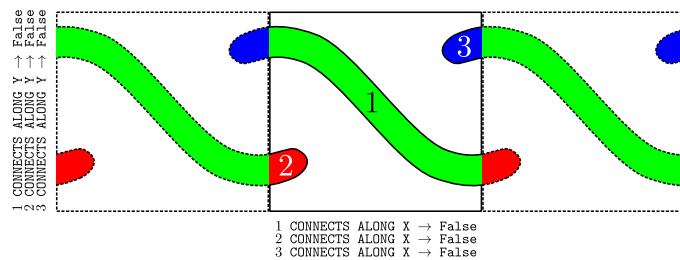
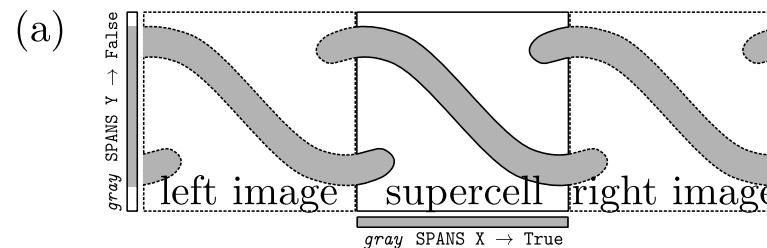
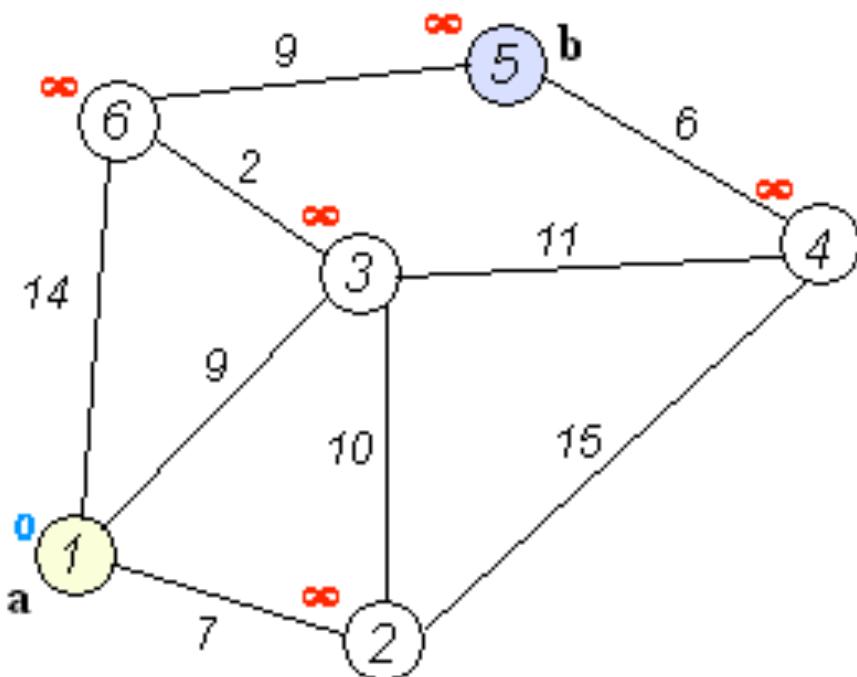


Existence of a Path is Insufficient

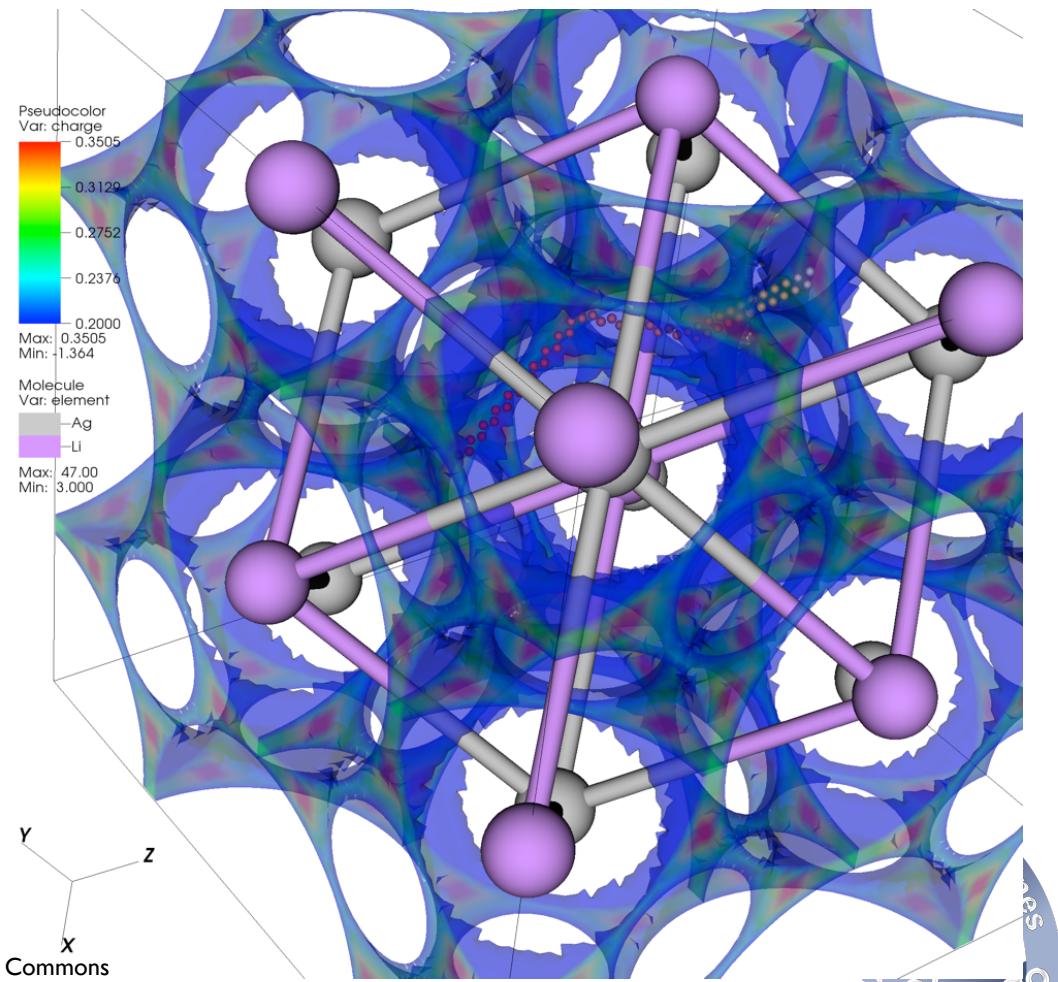


Dijkstra Path Identification Algorithm



brute force $\sim 10^{1,500,000}$ s
(age of the universe $\sim 10^{17}$ s)

DPI < 1 s



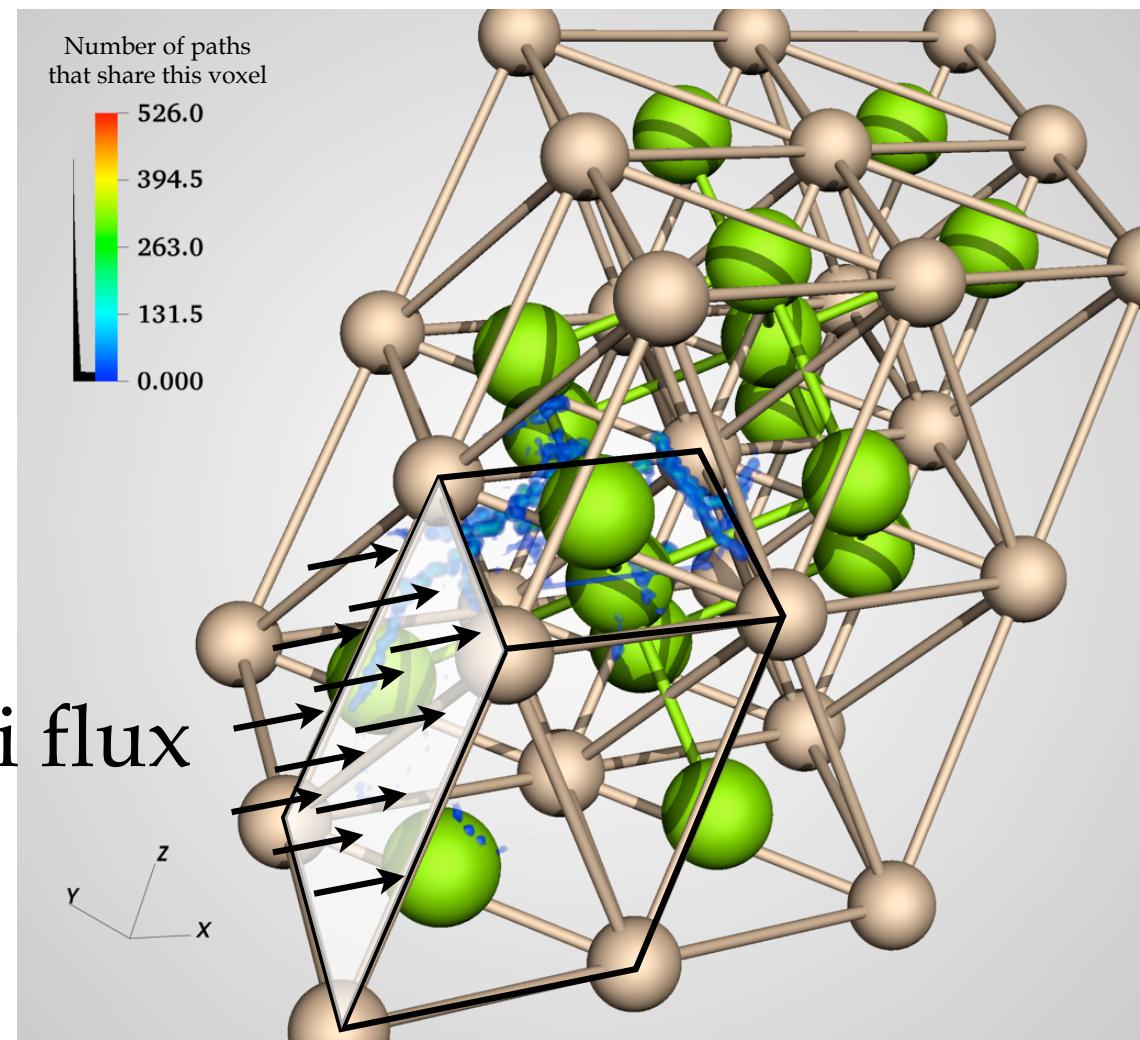
Path selection

Concept

Introduce a flux
along the a lattice
vector

Implementation

Find the low cost
path for over 2,000
start/end points



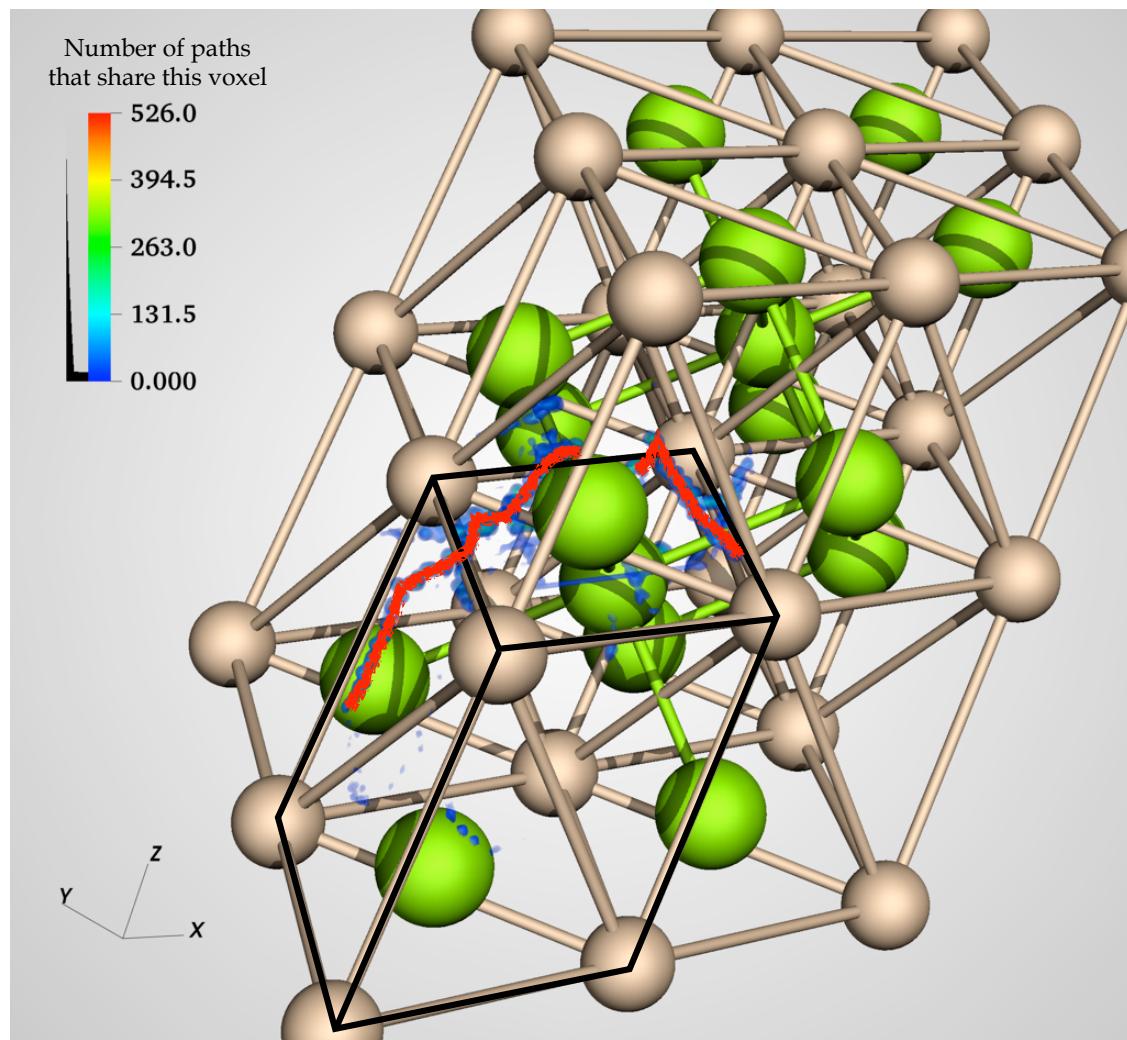
Path selection

Concept

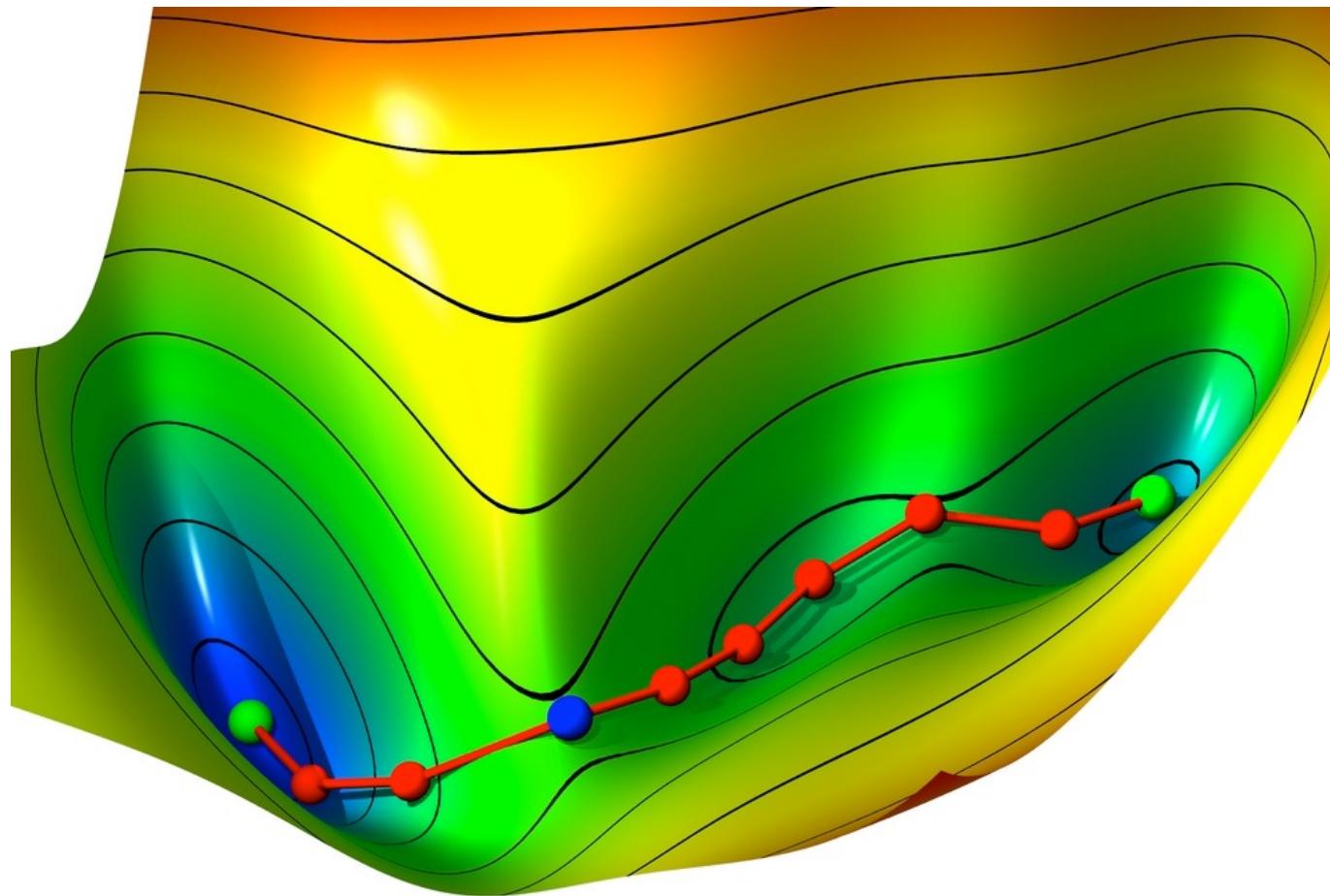
Introduce a flux
along the a lattice
vector

Implementation

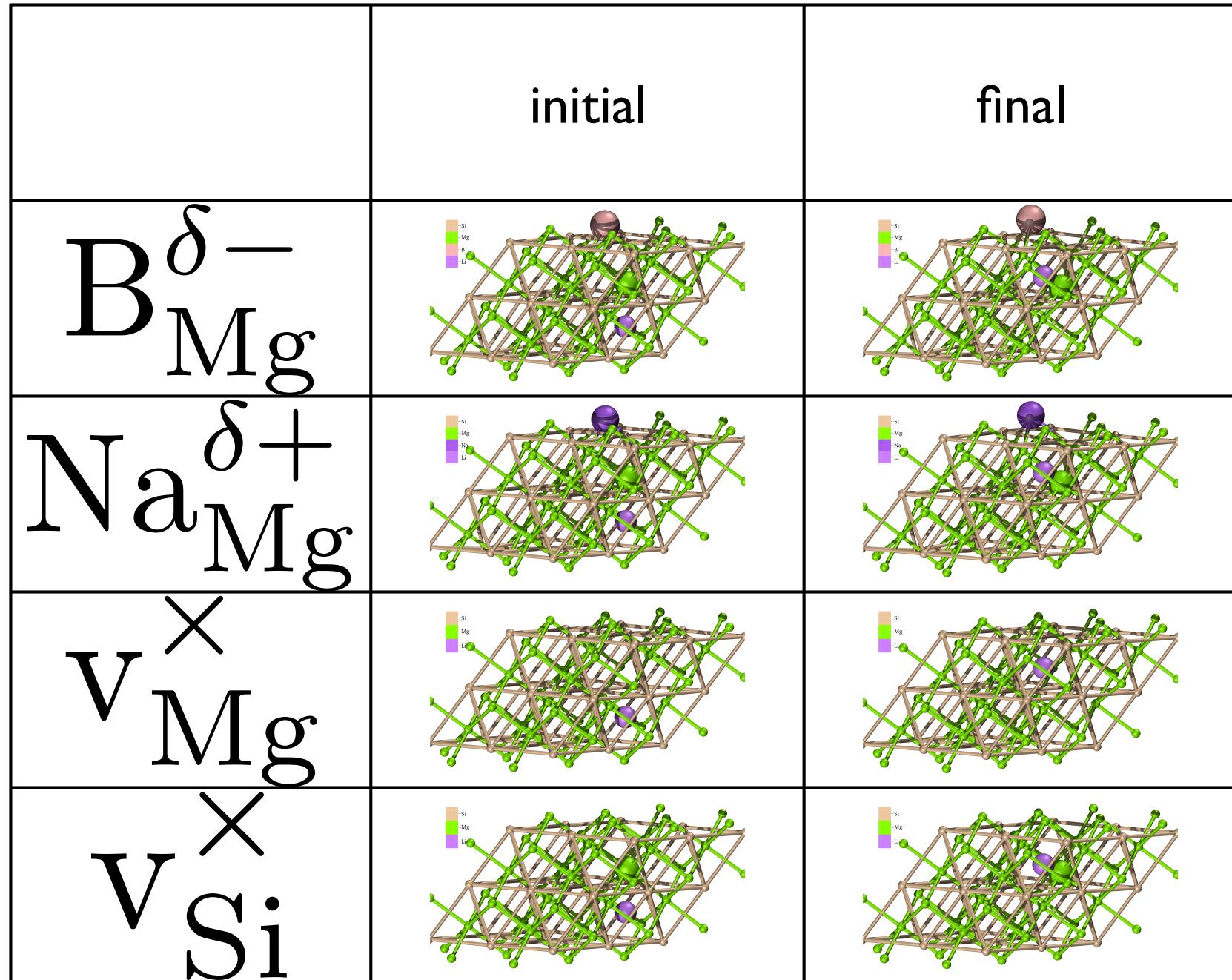
Find the low cost
path for over 2,000
start/end points



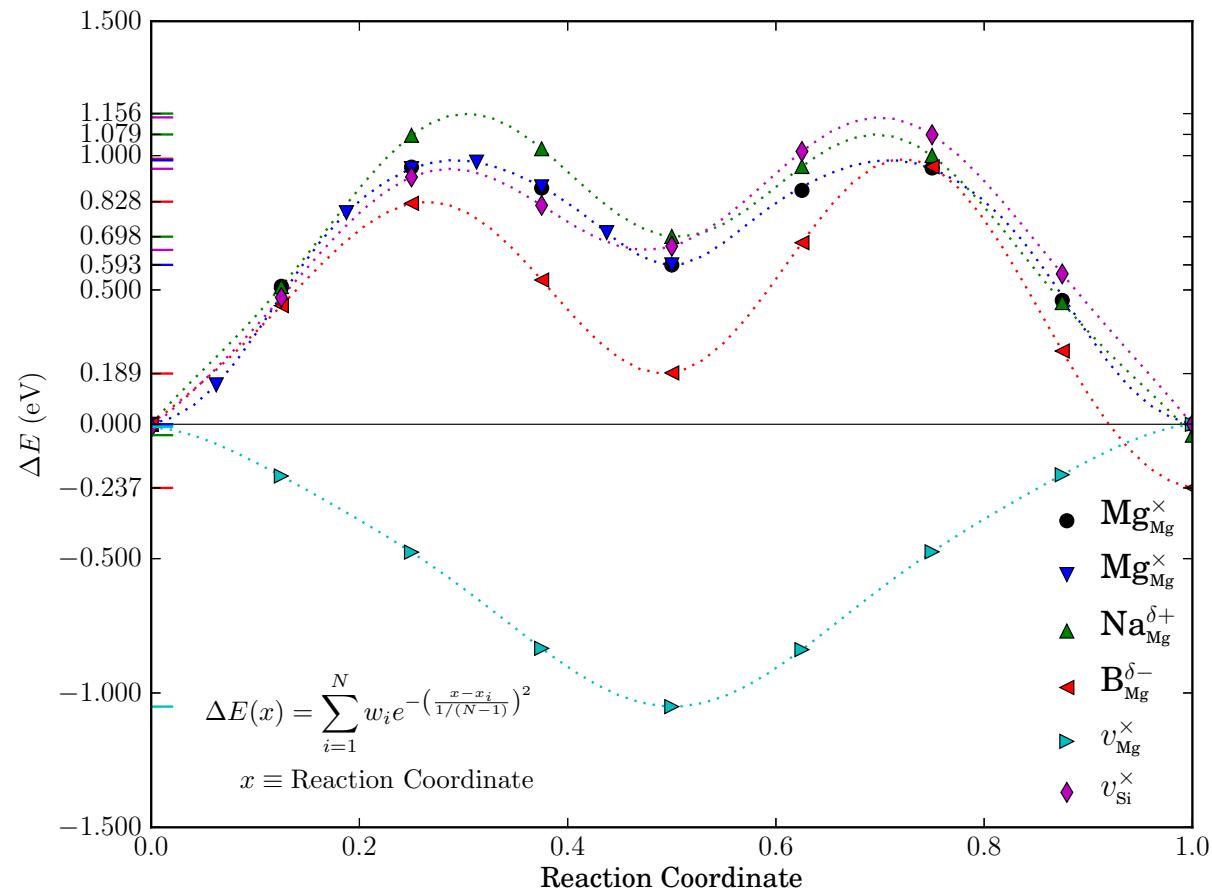
Nudged Elastic Band



Li-Mg₂Si Structures



Li-Mg₂Si Migration Enthalpies



Defect	Advancing Barrier (eV) Forward	Advancing Barrier (eV) Reverse	Metastable Energy (eV)	Retreating Barrier (eV) Forward	Retreating Barrier (eV) Reverse	ΔE (eV)
$\text{Mg}_\text{Mg}^\times$	0.976	0.383	0.593	0.383	0.976	0.000
$\text{Na}_\text{Mg}^\times$	1.156	0.458	0.698	0.381	1.120	-0.041
$\text{B}_\text{Mg}^\times$	0.828	0.639	0.189	0.799	1.225	-0.237
v_Si^\times	0.964	0.302	0.662	0.493	1.142	0.013
v_Mg^\times	0.302	0.493	-0.500	-0.500	-0.237	-0.237