

Chalcogen Chemistry and Cathodic Properties of Scandium-based Materials for Sodium-Ion Batteries

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Table S1. The optimized structure of $1 \times 1 \times 1$ of NaScO₂ has 12 atoms.

Na1 O2 Sc1

```
1.0000000000000000
3.1659998894000001 0.0000000000000000 0.0000000000000000
-1.5829999447000001 2.7418363326000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 16.2700004577999984
```

Sc Na O

3 3 6

Direct

```
-0.0000000000000000 -0.0000000000000000 0.0000000000000000
0.6666666870000029 0.3333333429999996 0.3333333429999996
0.3333333429999996 0.6666666870000029 0.6666666870000029
-0.0000000000000000 -0.0000000000000000 0.5000000000000000
0.6666666870000029 0.3333333429999996 0.8333333129999971
0.3333333429999996 0.6666666870000029 0.1666666719999981
-0.0000000000000000 0.0000000000000000 0.2650782326257056
0.0000000000000000 -0.0000000000000000 0.7349217973742898
0.6666666870000029 0.3333333429999996 0.5984115756257123
0.6666666870000029 0.3333333429999996 0.0682551033742899
0.3333333429999996 0.6666666870000029 0.9317448886257095
0.3333333429999996 0.6666666870000029 0.4015884243742877
```

Table S2. The optimized structure of $1 \times 1 \times 1$ of NaScS₂ has 12 atoms.

Na1 S2 Sc1

```
1.0000000000000000
3.7509999275000001 0.0000000000000000 0.0000000000000000
-1.8754999638000001 3.2484612267999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 19.7439994811999995
```

Sc Na S

3 3 6

Direct

```
0.0000000000000000 0.0000000000000000 -0.0000000000000000
0.6666666870000029 0.3333333429999996 0.3333333429999996
0.3333333429999996 0.6666666870000029 0.6666666870000029
0.0000000000000000 0.0000000000000000 0.5000000000000000
0.6666666870000029 0.3333333429999996 0.8333333129999971
0.3333333429999996 0.6666666870000029 0.1666666719999981
-0.0000000000000000 0.0000000000000000 0.2610758181178105
-0.0000000000000000 -0.0000000000000000 0.7389241818821896
0.6666666870000029 0.3333333429999996 0.5944091321178112
0.6666666870000029 0.3333333429999996 0.0722575168821885
0.3333333429999996 0.6666666870000029 0.9277425051178133
0.3333333429999996 0.6666666870000029 0.4055908378821863
```

Table S2. The optimized structure of $1 \times 1 \times 1$ of NaScSe₂ has 12 atoms.

Na1 Se2 Sc1

```

1.0000000000000000
3.9179999828000001 0.0000000000000000 0.0000000000000000
-1.9589999914000000 3.3930875172000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.7500000000000000
Se Sc Na
6 3 3
Direct
0.3333333429999996 0.6666666870000029 0.4270800050000005
0.6666666269999979 0.3333333129999971 0.5729199649999970
0.0000000000000000 0.0000000000000000 0.7604133489999967
0.3333333129999971 0.6666666269999979 0.9062533379999991
0.6666666870000029 0.3333333429999996 0.0937466700000016
0.0000000000000000 0.0000000000000000 0.2395866660000010
0.0000000000000000 0.0000000000000000 0.5000000000000000
0.6666666870000029 0.3333333429999996 0.8333333129999971
0.3333333429999996 0.6666666870000029 0.1666666719999981
0.6666666870000029 0.3333333429999996 0.3333333429999996
0.3333333129999971 0.6666666269999979 0.6666666269999979
0.0000000000000000 0.0000000000000000 0.0000000000000000

```

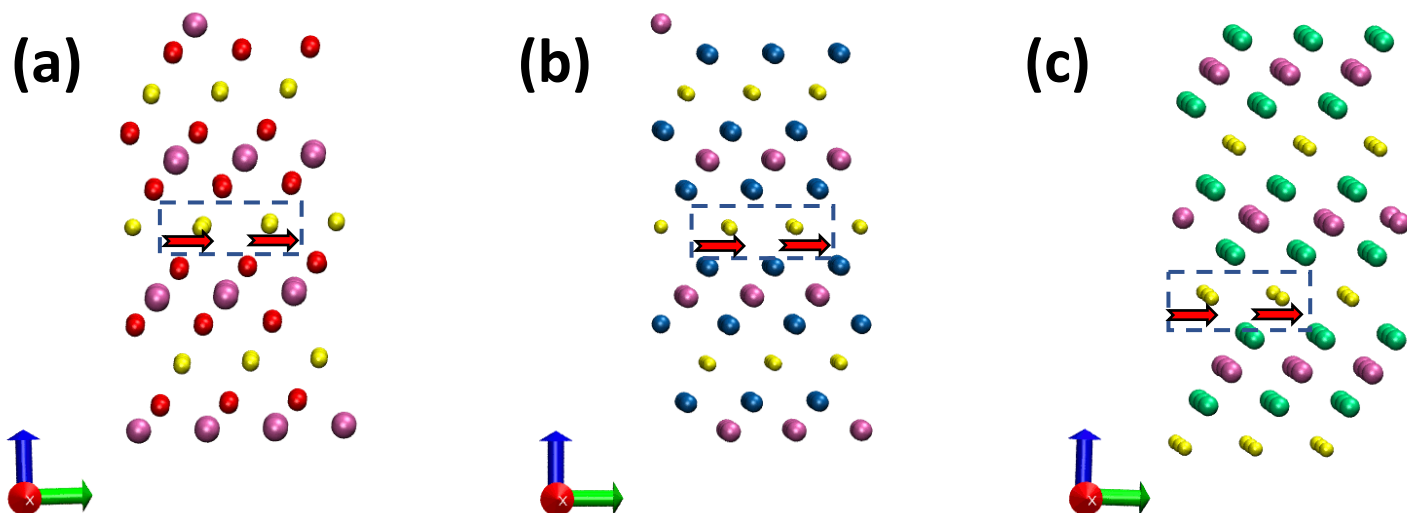


Figure S1. The animated view of the diffusion mechanism of (a) NaScO₂, (b) NaScS₂ and (c) NaScSe₂ along b axis (path-2).