Progress Report: Mechanism of lithium conduction in Li_xSi_y

immediate

July 1, 2022

1 Mechanism of lithium conduction in $Li_{13}Si_4$ and $Li_{12}Si_7$

- **First, we use the "reduce_trajec" script in order to obtain smaller trajectories which contain only every 100th or 10th frame.**
- **Second, we introduce a discrete lattice for the positions of the lithium atoms, suited for the description of the lithium conduction mechanism. In this study, we used the positions of the lithium atoms resulting from the relaxed crystal structures as lattice sites.**

1.1 Total jumps between lattice sites

The Figures in this section visualize the total number of ion jumps between the lattice sites (within the entire trajectory) by blue lines. The thickness of the lines is related to the number of ion jumps. The thickness is also normed with respect to the length of the trajectory and thus can be compared between different trajectories.

1.2 Total jumps between lattice sites in Li_13Si_4 at 500 K

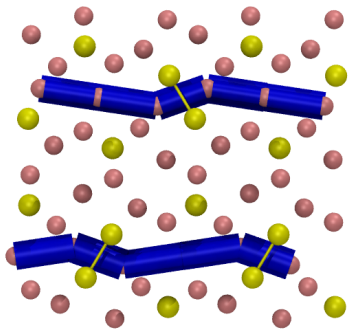

Figure 1: Total jumps between lattice sites in Li_13Si_4 at 500 K

```
cd PATH2/li13si4/elecell/500/get_jump_arrows
cp ../trajec/geo.xyz .
python create_lattice_unchanged.py
get_jump_arrows ../jump_mat.npy lattice_user_wrapped.npy geo_user_wrapped ../trajec/pbc_li13si4 1 1
vmd -e geo_user_wrapped.tcl
```

1.3 Total jumps between lattice sites in Li_13Si_4 at 800 K

```
cd PATH2/li13si4/elecell/800/get_jump_arrows
cp ../trajec/geo.xyz .
python create_lattice_unchanged.py
get_jump_arrows ../jump_mat.npy lattice_user_wrapped.npy geo_user_wrapped ../trajec/pbc_li13si4 1 1
vmd -e geo_user_wrapped.tcl
```

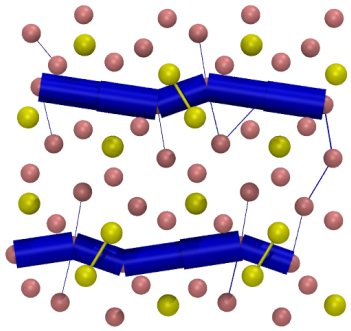

Figure 2: Total jumps between lattice sites in Li_13Si_4 at 800 K

1.4 Total jumps between lattice sites in Li_12Si_7 at 500 K

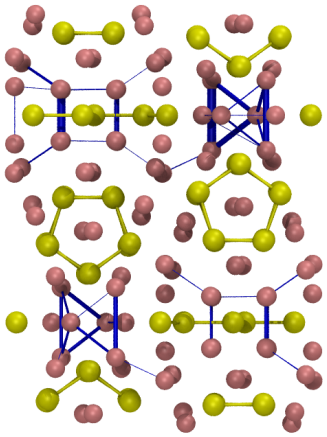

Figure 3: Total jumps between lattice sites in Li_12Si_7 at 500 K

```
cd PATH2/li12i7/elecell/500/get_jump_arrows
cp ../trajec/geo_new.xyz .
get_jump_arrows ../jump_mat.npy ../lattice1.npy geo_new ../trajec/pbc_li12si7 1 1
vmd -e geo_new.tcl
```

1.5 Total jumps between lattice sites in Li_21Si_5 at 500 K

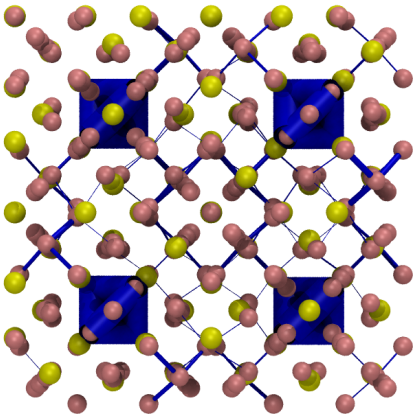

Figure 4: Total jumps between lattice sites in Li_21Si_5 at 500 K

```
cd PATH2/li21si5/elecell/500/get_jump_arrows
cp ../trajec/geo_new.xyz .
get_jump_arrows ../jump_mat.npy ../lattice1.npy geo_new ../trajec/pbc_li21si5 1 1
vmd -e geo_new.tcl
```

1.6 Total jumps between lattice sites in Li_17Si_4 at 800 K

```
cd PATH2/li17si4/elecell/500/get_jump_arrows
cp ../trajec/geo_new.xyz .
get_jump_arrows ../jump_mat.npy ../lattice1.npy geo_new ../trajec/pbc_li21si5 1 1
vmd -e geo_new.tcl
```

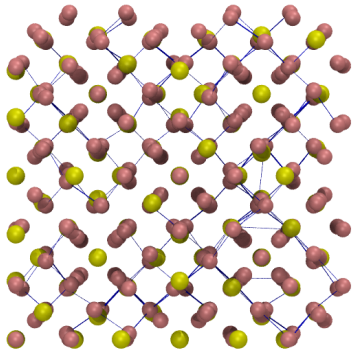

Figure 5: Total jumps between lattice sites in Li_17Si_4 at 800 K

1.7 Total jumps between lattice sites in Li_22Si_5 at 500 K

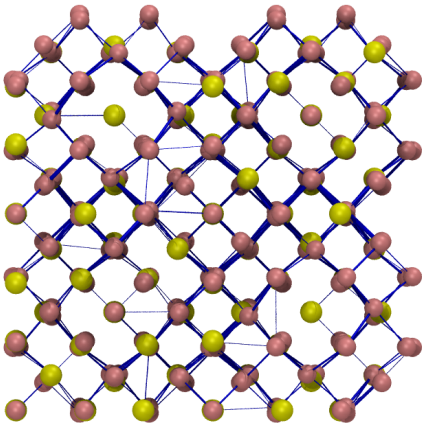

Figure 6: Total jumps between lattice sites in Li_22Si_5 at 500 K

```
cd PATH2/li22si5/elecell/500/get_jump_arrows
cp ../trajec/geo_new.xyz .
get_jump_arrows ../jump_mat.npy ../lattice1.npy geo_new ../trajec/pbc_li22si5 1 1
vmd -e geo_new.tcl
```

1.8 SDF of all lithium atoms

Only on principal example because i believe that this function is not so important.

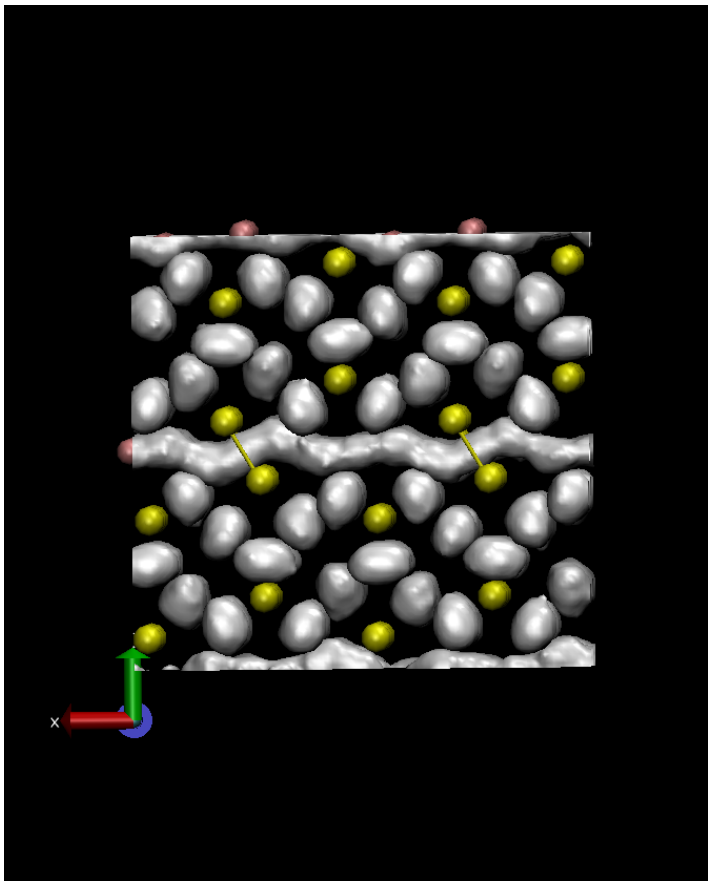

Figure 7: SDF of all lithium atoms Li_13Si_4 at 500 K

```
cd PATH2/li13si4/elecell/500/cube_and_saddle_smooth
python cube_and_saddle_smooth.py
vmd  full_dens_smooth1.cube
save manually to file
```

1.9 Averaged lithium fluxes

1.9.1 Which scripts were used to produce these figures or tables:

- **create_jump_mat_li**
- `special_sdf.py`
- vmd

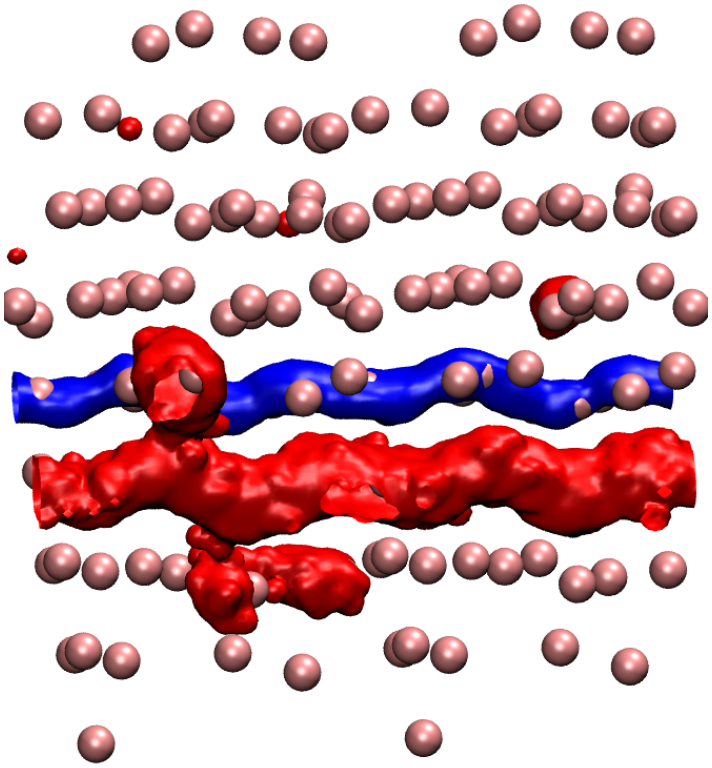

Figure 8: Spatial density/averaged fluxes of lithium atoms in li13si4, which start from a specific lattice site. Blue: 500K, red: 800K.

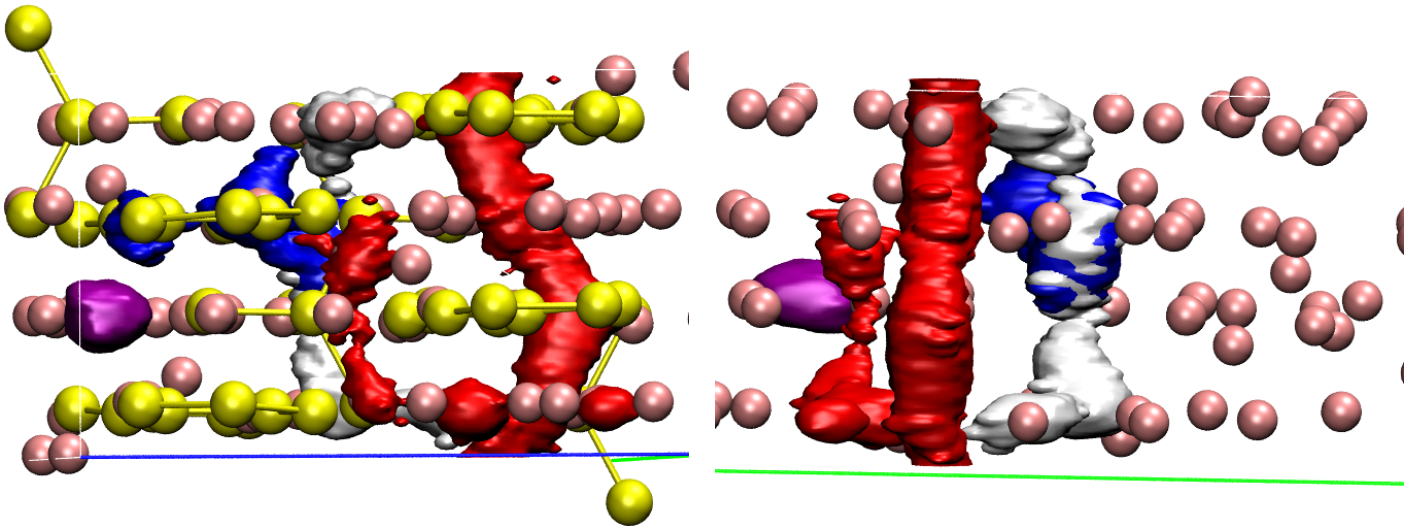

Figure 9: Spatial density/averaged fluxes of lithium atoms in li12si7, which start from a specific lattice site. Different colors indicate different initial lithium sites.

1.10 Statistical analysis of connected jumps

- Within a given temporal interval (x-axis in the Figures 10 and 11), we determine groups of lithium sites which are connected by lithium jumps. These groups of connected lithium sites are referred to as jump types.
- Within our statistical analysis of the connected jumps, we determine the different jump types as well as their occurrence.

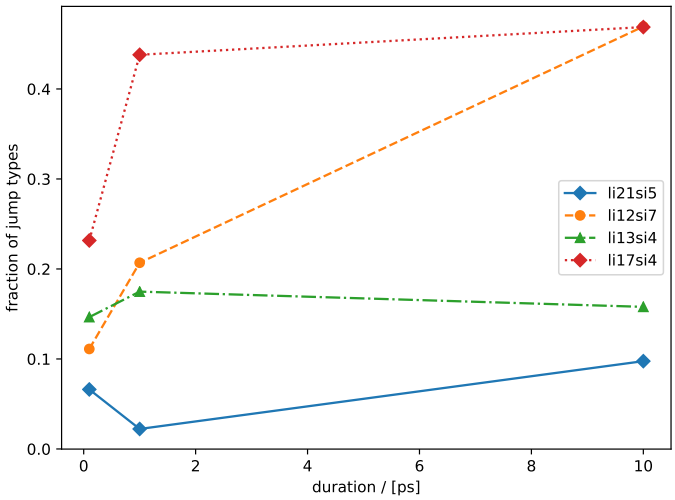

Figure 10: We determined the number of lithium jump types which contribute 50 % to the overall number of lithium jumps. In this Figure, the ratio between this number and the overall number of detected jump types is presented with respect to different maximal durations of a lithium jump. Be careful li17si4 is investigated at 800K!

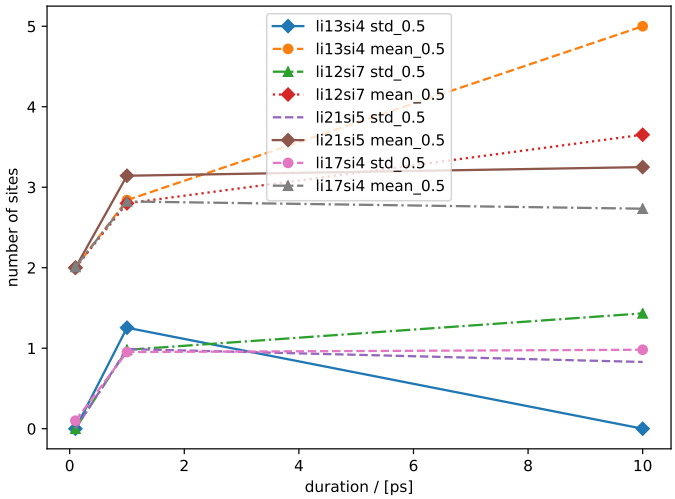

Figure 11: We determined the number of lithium jump types which contribute 50 % to the overall number of lithium jumps. In this Figure we analyse the most frequent lithium jump types which contribute 50 % to the overall number of lithium jumps. We calculated the average and the standard deviation of the number of lithium sites, which are involved in these jump types.Be careful li17si4 is investigated at 800K!

1.10.1 Which scripts where used to produce these figures or tables:

- **create_jump_mat_li**
- jumps_from_grid ../jump_mat.npy 0 1500 1 1
- cp jump_hist.txt jump_hist_1.txt

- jumps_from_grid ../jump_mat.npy 0 1500 10 10
- cp jump_hist.txt jump_hist_10.txt
- jumps_from_grid ../jump_mat.npy 0 1500 100 100
- cp jump_hist.txt jump_hist_100.txt
- prepare dicts with statistic data
  - `$PATH2/li13si4/elecell/500/advanced_jump_stat_ready_to_print/advanced_jump_stat_ready_to_print.py`
  - `$PATH2/li12si7/elecell/500/advanced_jump_stat_ready_to_print/advanced_jump_stat_ready_to_print.py`
  - `$PATH2/li21si5/elecell/500/advanced_jump_stat/advanced_jump_stat_ready_to_print.py`
  - `$PATH2/li15si4/elecell/800/advanced_jump_stat/advanced_jump_stat_ready_to_print.py`
  - `$PATH2/li17si4/elecell/800/advanced_jump_stat/advanced_jump_stat_ready_to_print.py`
- plot dicts to Figure:
  - `/net/shared/dressler/creating_nice_figures_2018/lithium/jump_stat2/plot_dict1.py`
  - `/net/shared/dressler/creating_nice_figures_2018/lithium/jump_stat2/plot_dict_avg_std.py`
  - `/net/shared/dressler/creating_nice_figures_2018/lithium/jump_stat2/test.py`

compound	number of Li jumps
li21si5	7725
li15si4 800 K	12
li12si7	1114
li13si4	5387
li22si5	7810
li17si4 800 K	997

Table 1: Number of total Li jumps NOT normalized by number of Li lattice sites or the trajectory length. A connected jump between three lithium sites is counted as only one jump.

1.11 Sequential or concerted lithium jumps?

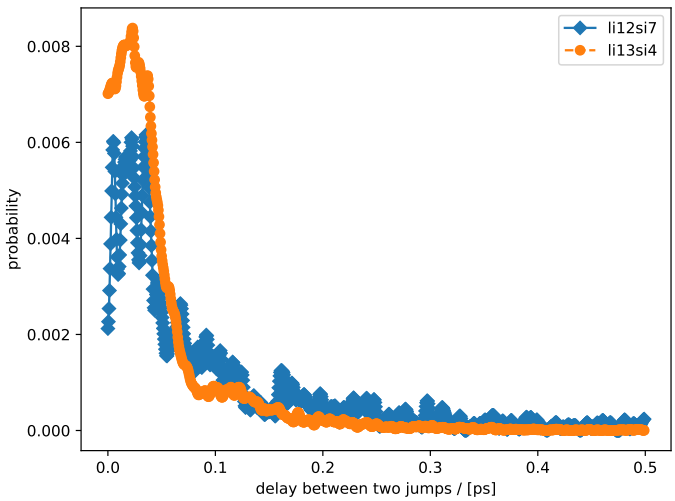

Figure 12: We present a probability distribution of the delay between lithium jumps between lattice sites in direct spatial adjacency.