**Specific Question:**

We want to build the relation chain from diffusion coefficient D 🡪 activation energy EA 🡪 hopping length L 🡪 structure data

From POWGEN structure analysis (at 300K) we got the Li 🡪 Li site distances. I determined them for all three structures (tetragonal LLZO, 36Al-LLZO and 60Ta-LLZO) with Diamond 4 crystal structure software, so we can compare them.

I read about Chudney-Elliot Equation (CEEq) in Hempelmann’s book “*QENS and solid state diffusion”* [year 2000] (p. 118-119) that CEEq is useful for calculation the Diffusion coefficient at large Q-values (>1 Å-1) and that for small Q-values Fick’s 1st law (F1stL) can be used. This is basic we all know.

As I noticed that the jump distance L can be determined by Fick’s 1st Law, too, that makes everything a little bit easier for us, as we only work at small Q-range of 0.3-1.1 Å-1.

The residence time **τ** can be determined by the equation, with **τ0**the pre-exponential factor:

**Now the question:**

To determine the jump/hopping distance L, we need the residence time **τ**. How do we get this residence time value, or the pre-exponential factor **τ0**?

Maybe Robert knows the answer, as he calculated it in his draft paper?

The residence time should in principle come directly from the fit of HWHM over the whole range of Q, including high Q as we discussed during the experiments. I know we limited ourselves to 1.1 A-1 in the fits due to coherent peaks at high Q.

Note however, that for long range translational diffusion as seems to be the case in your systems (and not in the amorphous LiSi Sacci measured), tau becomes infinitely small and can not be calculated a Li does not reside long enough in any site. Perhaps we should plot data over whole Q range to see …

Assuming we can pull all tau vs T, then the pr-efactor comes simply from fitting the Arrhenius expression you wrote above.

Now perhaps, you could use your estimated jump length from POWGEN to estimate the tau values, (tau=D/6l) if you assume hopping mechanism.