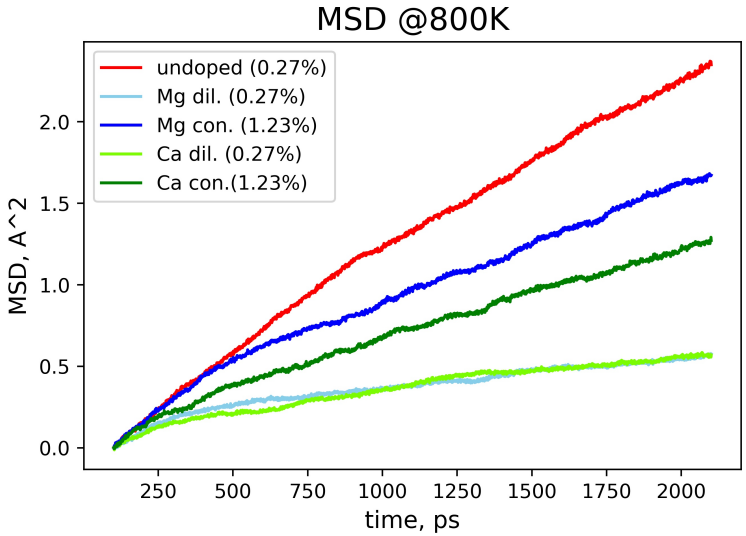
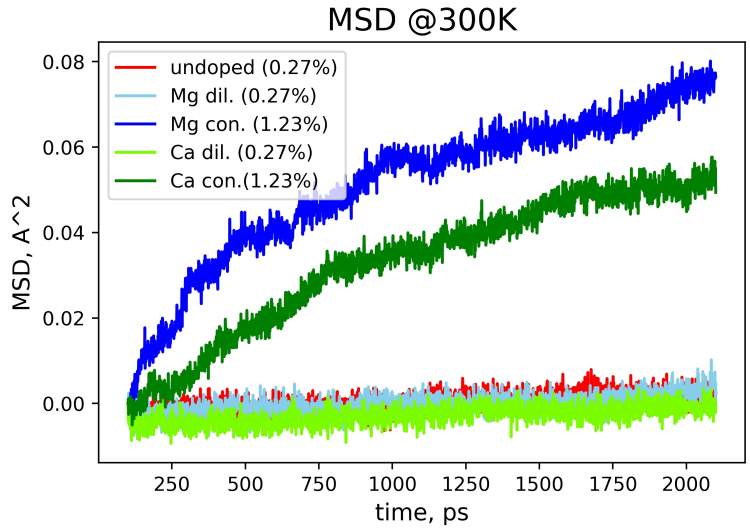
April Update

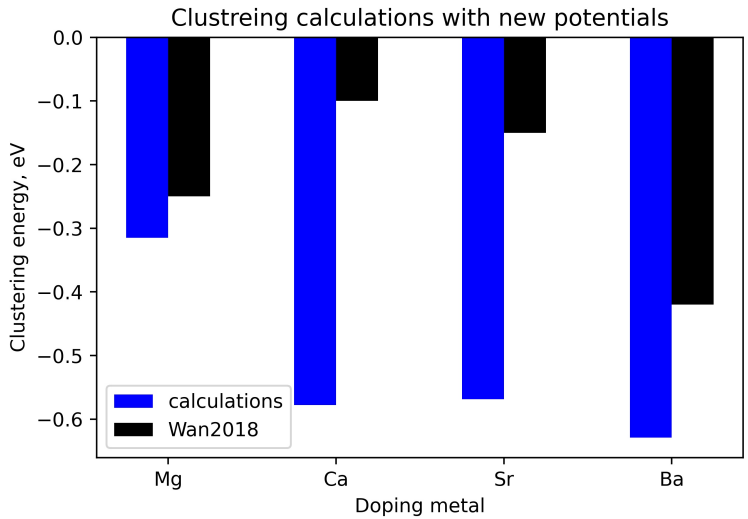
Ben Goldmann

April 14, 2021

15x15x15 supercell for 2ns







Diffusion coefficients

structure	**300K, m2/s**	**800K, m2/s**
undoped	2.68e-17	1.15e-14
0.27% Mg doped	2.59e-17	2.26e-15
1.23% Mg doped	2.90e-16	7.70e-15
0.27% Ca doped	2.53e-17	2.55e-15
1.23% Ca doped	2.68e-16	5.90e-15

Halospinel modelling

- the search for Sc-Cl potential
  - found a Born-Mayer potential from 2009
  - can use these numbers after some algebraic adjustment?
- structural questions
  - random (these sites are all equivalent) positions of Sc in 1/3 of the spinel-like (spl) octahedral sites (1/2 of total octahedral sites are spl, so 1/6 of octahedral sites filled with Sc)
  - random (as "Li site energies are relatively similar") positions of Li in remaining 2/3 spl octahedral sites (2/6 of tot oct), spl tetrahedral sites (1/8 of tot tet), non-spl octahedral sites (3/6 of tot oct) and non-spl tetrahedral sites (7/8 of tot tet)
  - taking 3 unit cells: of the possible Sc sites (6) 2 occupied; after this of the possible Li sites (34) 6 occupied
  - ASSUMPTION: Li can be in any tetrahedral hole even in those where all 4 sides are face-sharing with spl octahedra (3 of these in above example, 3 of them don't share any faces - these are the spl tetrahedrals, remaining 18 share 2 faces with spl octahedra)