The interaction pair potential between ions i and j consists of a short-range term, the long-range Coulombic term and van der Waals interactions. These short-range interactions were modeled using the Buckingham potential:

\[ V_{ij}(r_{ij}) = A \exp(-r_{ij}/r) - C r_{ij}^2 \quad \text{Eq. 1} \]

Where A, F, and C are the Buckingham potential parameters and r is the interatomic distance. Figure 1 depicts the supercell as well as the unit cell of a lithium cobalt oxide cathode materials.

The interaction potential between the ions can be written as:

\[ V_{ij}(r_{ij}) = A \exp(-r_{ij}/r) - C r_{ij}^2 \quad \text{Eq. 1} \]

Where A, F, and C are the Buckingham potential parameters and r is the interatomic distance. Figure 1 depicts the supercell as well as the unit cell of a lithium cobalt oxide cathode materials.

**Results and discussion**

**Structural parameters**

The structure of LiCoO\(_2\) at the equilibrium state was measured by the radial distribution function (RDF).

- These peaks are sharp at low temperatures and become broad at higher temperatures which is due to thermal motion.
- The height of the first peak decreases as the temperature increases because ions move away from equilibrium lattice positions at high temperatures and the crystalline volume expansion.

**Mean square displacement**

The mean square displacements (MSD) as a function of time for each species were calculated to investigate the diffusive properties of each species.

- The MSDs reach a constant value after a relaxation time.
- The mobility of lithium ions is anisotropy because lithium ions are less mobile in the Z direction comparing to that of Y and X directions.

**Conclusions**

- Lithium ions are more thermally activated compared to those of oxygen and cobalt ions.
- Lithium ions have higher MSD comparing to those of oxygen and cobalt ions.
- Radial distribution function of different ions shows as the temperature increases, the degree of disorder in the crystalline lattice increases especially at higher temperatures.
- Higher lattice distortion and expansion causes the reduction of thermal transport at higher temperatures.
- Using partial phonon density of states, the contributions of the various species on the phonon DOS were differentiated showing that lithium ions have more vibrations in all different directions rather than oxygen and cobalt ions.

**References**


