Solvation of Li^+ and Na^+ in cyclic and linear carbonate based battery electrolytes

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Sodium-ion batteries are currently a scientific field under rapid development and thus there is a need to also understand and study electrolyte materials for use in such batteries.

The solvent commonly used for Li-ion batteries is a mixture of ethylene carbonate (EC) and dimethyl carbonate (DMC). This combination is therefore a convenient starting point to study the solvation of Na^+ for Na-ion batteries (even if the final optimized solvent combination may be another).

Here the $Na(EC)_x(DMC)_y^+$ system is studied by using density functional theory (DFT). As a comparison $Li(EC)_x(DMC)_y^+$ is also studied.

The systems had their configuration space mapped with high throughput DFT calculations to identify the most likely coordination structures for the two central alkali cations. This involved a GPU enabled program and the B3LYP/6-31G basis set with and without dispersion correction to the DFT approach.

The x+y=4 case, *i.e.* the tetrahedral structure, was then studied in further detail with a larger basis set and an additional functional. This was both to improve the results and to explore the details of the solvation structure.