MD-Simulations on polysulfide – electrolyte- interactions in solid state batteries
(In Cooperation with Georg Garnweitner in the SE2A cluster of excellence)

Problem:
The migration of the polysulfides through the electrolyte represents one of the greatest challenges in the development of lithium-sulfur batteries, as this results in a steady loss in capacity and shorter lifetime. Novel solid-state electrolytes or hybrid electrolytes that are developed in the SE2A project C2.3 therefore require components or functional groups that show a high affinity (binding energy) for polysulfides in order to minimize the migration. A targeted improvement of the electrolyte can be realised by determining the interaction of different polysulfides and the electrolyte by MD simulations. This allows the prediction of the electrolyte ability to suppress the polysulfide migration - without the need to conduct time consuming electrochemical experiments.

In this student project, the following MD studies shall be performed

- Diffusivity of different polysulfides through the electrolyte (pentaerythritol tetraacrylate, PETEA).
- Structural analysis (RDFs etc) to identity interaction pattern between the polysulfides and functional groups of the electrolyte
- Yield information how a variation of functional groups can enhance the binding of the polysulfides to the electrolyte to minimize migration