DOCTORAL CANDIDATE:	Raphael Mathias Peltzer
DEGREE:	Philosophiae Doctor
FACULTY:	Faculty of Mathematics and Natural Sciences
DEPARTMENT:	Department of Chemistry
AREA OF EXPERTISE:	Theoretical and Computational Chemistry
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DISSERTATION TITLE:	*Multi-scale computational modelling of bio-chemical systems in the condensed phase*

The number of bio-chemical systems and processes that are able to be modeled and understood using computational chemistry tools and the boundaries of feasible simulations are constantly extended. In his thesis, Raphael Peltzer, a PhD-Scholar from the University of Oslo, uses state-of-the-art computational chemistry tools better understand reactions in both organic chemistry and biochemistry and how these tools can help us solve old problems as well as help the advance of present day research.

He was able to show how the solvent influences the constitution of the Grignard reagent in the so-called Schlenk-Equilibrium reaction. Understanding this equilibrium is key to fully characterizing the Grignard reagent, a textbook organic chemistry reaction that has been recognized with the Noble Prize in Chemistry in 1912 and whose reagents are to this date used in large-scale industrial chemistry processes. His research brings us 1 step closer to finally fully understanding this reaction and might aid the design of future metallo-organic synthesis.

In his thesis, he also shows how we can use the predictive power of computational chemistry to understand and characterize frontier research. He was able to simulate the assembly process of small protein monomers into larger spherical nanoparticles, which had been found and characterized recently by experimental researchers at the University of Bern. The researchers furthermore found that this protein, that is a key component in the uptake of Vitamin E into the human body, might have further reaching functionalities in the human body, including influence on the development of the early nervous system in embryos and enhanced transport properties inside the body. The characterization of the assembly process on the one hand made it possible to predict the influences of modifications to the protein on its assembly process and structure. On the other hand it might aid the drug design linked to this protein and its intriguing nanoparticle assembly in the future.