Computational Materials Science: Where Theory meets Experiment (1500char total)

In contemporary materials research, we are able to create and manipulate materials at ever smaller scales: the growth of wires with nanoscale dimensions and the deposition of layers with a thickness of only a few atoms are just two examples that have become common practice. At this small scale, quantum mechanical effects become important, and this is where computational materials research comes into play. Using clever approximations, it is possible to simulate systems with a scale relevant for experiments. The resulting theoretical models provide fundamental insights in the underlying physics and chemistry, essential for advancing modern materials research. As a result, the use of computational experiments is rapidly becoming an important tool in materials research both for predictive modeling of new materials and for gaining fundamental insights in the behavior of existing materials. Computer and lab experiments have complementary limitations and strengths; only by combining them can the deepest fundamental secrets of a material be revealed.

In this presentation, we focus on the application of computational materials science for ceramic materials, nanowires on semiconductor surfaces, and flexible metal-organic frameworks.