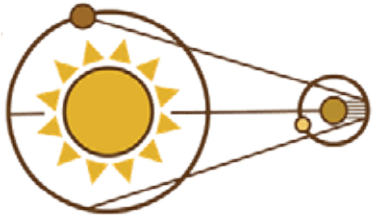
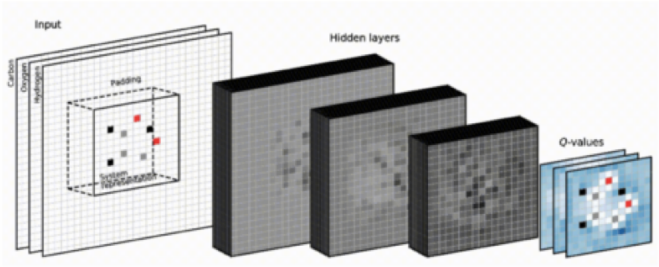
Aarhus University presents

The Ole Rømer Colloquium Series





Wednesday, October 12th @ 14:15 (sharp!)
Physics Auditorium (1523-318)

Professor Bjørk Hammer

Department of Physics & Astronomy,
Aarhus University

On the use of Machine Learning in Computational Chemistry and Materials Science

Recently, researchers in the field of computational chemistry and materials science have realized that the highly complex and computationally expensive data they produce on super computers may be used to train machine learning models. Depending on the amount and type of data used, the models may become highly accurate and hence alleviate the need for further expensive computations at the first-principles level. In the presentation, it will be discussed how molecular and crystalline structures must be represented to enable machine learning of the underlying interaction potentials. Gaussian Process Regression and artificial neural networks will be introduced for the models, and adaptive and reinforcement learning protocols will be used to construct machine learning models that reveal new molecular cluster shapes and new reconstructions for crystalline surfaces.

Students & staff are all invited!

14:00-14:15: Informal discussions, cake & coffee
14:15-15:15: Seminar and Q&A
15:15-15:45: Special session between students & speaker