Speaker: **Michael Streif**

Title: **Quantum computing in the pharmaceutical industry**

Place: **Room 915 and Zoom (Information will follow)**

Abstract:

Drug discovery is often mentioned as one of the future application fields of quantum computers. In the first part of my talk, I will motivate how the pharmaceutical industry could benefit from quantum computing and explain why it is nevertheless hard to find good quantum computing use cases. In the second part, I will talk about the calculation of molecular forces [1] and introduce novel quantum algorithms for noisy intermediate scale (NISQ) and fault tolerant (FTQC) quantum computers, with substantially reduced cost compared to previous methods. Our results suggest that the calculation of forces has a similar cost to estimating energies of chemical systems. However, since molecular dynamics simulations typically require 10^6-10^9 unique force calculations, current known methods for MD on quantum computers are impractical and new approaches need to be found.

[1] O'Brien, T. E., Streif, M., Rubin, N. C., Santagati, R., Su, Y., Huggins, W. J., ... & Babbush, R. (2021). Efficient quantum computation of molecular forces and other energy gradients. *arXiv preprint arXiv:2111.12437*.