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Theoriekolloquium

Jan. 14, 2021 at 4 p.m. usually Newton-Raum, Staudinger Weg 9, 01-122

Dries Sels New York University

Quantum assisted compound identification for NMR spectroscopy

Recent technological advances have put us at the brink of having access to small scale quantum computers capable of solving problems that cannot be tackled with classical computers. A limited number of algorithms have been proposed and their relevance to real world problems is a subject of active investigation. Solving problems relevant to chemistry are expected to be the first successful applications of quantum computers. In this talk, I will discuss a particular problem that can be solved efficiently on quantum computers: model inference for nuclear magnetic resonance (NMR) spectroscopy. I will give a broad introduction to quantum computing and NMR metabolomics assuming no prior knowledge of the subject.