Bridging Orthogonal Worlds: Computational Chemistry as a Trading Zone between Quantum Foundations and Big Data

Chemistry is currently undergoing one of the most fundamental transformations in its history. The field has always been shaped and driven by countless experimental observations—a context that lends itself to analysis with machine learning methods. It is therefore not surprising that agentic artificial intelligence is increasingly gaining ground, simplifying and automating experimental and computational workflows. At the same time—albeit somewhat more slowly due to hardware limitations—we are witnessing the rise of quantum computation as a new computing paradigm, with chemistry and materials science as its key areas of application. Naturally, concepts from quantum information theory and novel algorithmic approaches are being integrated into the classical quantum mechanical foundations of chemistry; this not only yields new insights and ideas but also transforms our understanding of traditional quantum chemical concepts and methods. In less than a decade, we have now entered what Peter Galison calls a "trading zone": a highly dynamic melting pot that amalgamates exciting recent developments in computation to create a new kind of chemistry. In my lecture, I will address these developments and illustrate them with examples.