Have you ever pulled on a molecule? - Chemical Reactivity by Interactive Quantum Mechanics

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IQCC Seminar
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Location: GoToMeeting

Our capability to describe molecular structures based on the first principles of quantum mechanics has reached a breathtakingly high degree of sophistication, maturity, and feasibility. At the same time, theoretical chemistry as a research field has diversified dramatically over the years. Significant progress has been made in all its diverse subfields. Its capabilities as well as the open challenges are very well understood. Moreover, many unexpected new concepts - in electronic structure theory, vibrational spectroscopy, data-driven chemistry, quantum information and quantum computing, etc. - developed in the past twenty years highlight the enormous current impetus and momentum of the field.
In my talk, I will reflect on some of these developments and then focus on our new concept of real-time quantum chemistry that allows one to get immersed into molecular reactivity through interactive quantum mechanics.