

Mary E. Kapp Lecture in Chemistry

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"Nothing Amuses More Harmlessly Than Computation ..."

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Over the past two decades or so, computational studies of classical and quantum phenomena have taken their rightful place alongside experiment and theory as important probes of physical and chemical phenomena. Via selected examples, I will review some of the progress, especially as it applies to chemistry, and materials science. The talk will also highlight some challenges and opportunities for computational studies in the coming decade arising from the marriage of the physical and life sciences.