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Title: Mapping Atomic Motions with Ultrabright Electrons: Realization of the Chemists' Gedanken Experiment
Date: Thursday, December 8, 2016
Time: 4pm
Venue: AG-69, TIFR, Homi Bhabha Road, Colaba, Mumbai

Abstract:
One of the grand challenges in science has been to watch atomic motions during structural transitions, i.e. watch atomic motions in real time. Due to the extraordinary requirements for simultaneous spatial and temporal resolution, it was thought to be an impossible quest and has been previously discussed in the context of the purest form of a gedanken experiment. With the recent development of ultrabright electron sources capable of literally lighting up atomic motions, this experiment has been realized (Siwick et al. Science 2003). Increased source brightness, has enabled the study of photoinduced intermolecular charge transfer process in organic systems (Gao et al Nature 2013), as well as cyclization reactions with bond formation and conserved stereochemistry used in synthetic strategies (Jean-Ruel et al JPC B 2013). One observes the innumerable possible nuclear motions collapse to a few key reaction modes. Even more dramatic reduction in complexity has been observed for the material, Me4P[Pt(dmit)2]2, which exhibits a photo-induced metal to metal electron transfer process. This study represents the first full atom resolved structural dynamics with sub-Å and 100 fs timescale resolution (Ishakawa et al Science 2015). At this resolution, without any detailed analysis, the key large-amplitude modes can be identified by eye. We now are beginning to see the underlying physics for the generalized reaction mechanisms that have been empirically discovered over time. The "magic of chemistry" is this enormous reduction in dimensionality, due to the extremely large anharmonicity in the barrier crossing region, that ultimately makes chemical concepts transferable. How far can this reductionist view be extended with respect to complexity? In this respect, atomically resolved protein functions provide a definitive test of the collective mode coupling model (Miller Acc. Chem. Research 1994) to bridge chemistry to biology, which will be discussed as the driving force for this work.