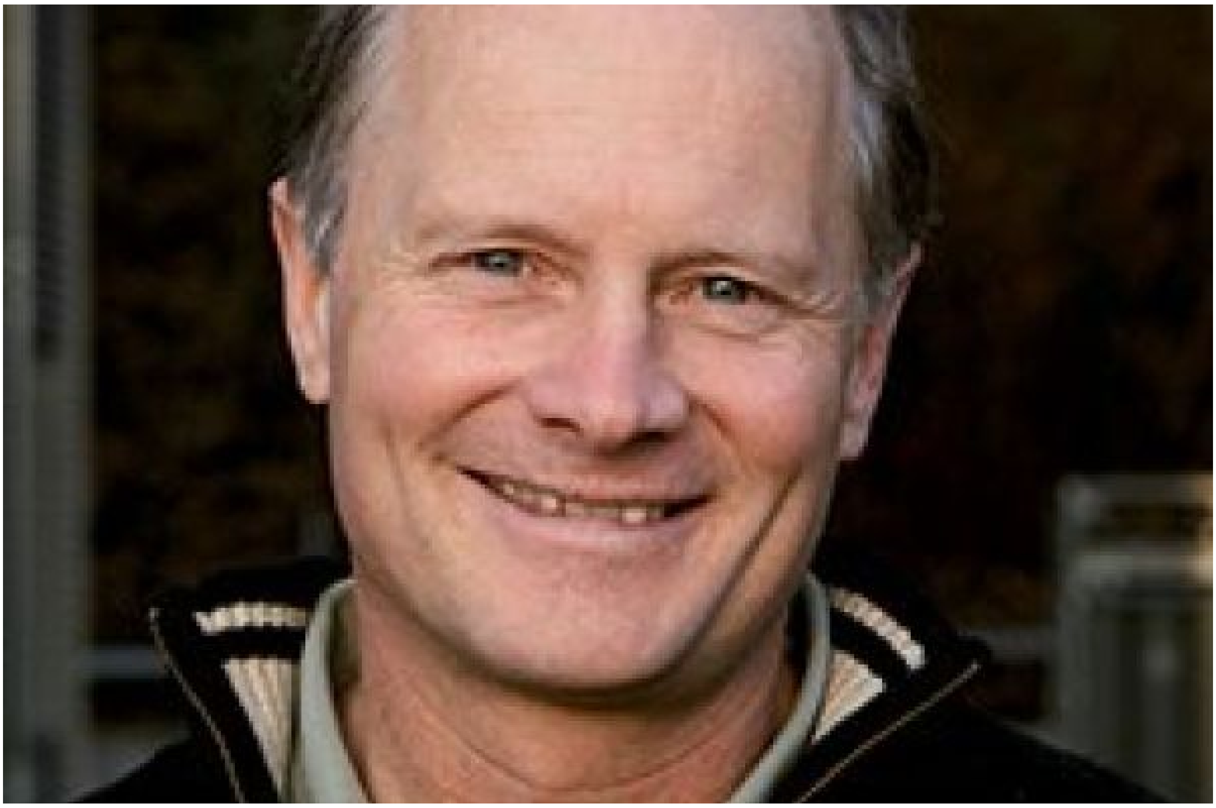

ICFO COLLOQUIUM R. J. DWAYNE MILLER 'Mapping Atomic Motions with Ultrabright Electrons: Fundamental Space-Time Limits to Imaging Chemistry and Biological Processes'

R. J. DWAYNE MILLER

April 05, 2019

Friday, April 5, 2018, 12:00. ICFO Auditorium

R. J. DWAYNE MILLER

Director of the Atomically Resolved Dynamics Division The Max Planck Institute for the Structure and Dynamics of Matter and Professor of Chemistry and Physics, Distinguished Faculty Research Chair in Chemical and Biological Physics University Professor University of Toronto
$$R. J. Dwayne Miller has published over 200 research articles, one book, and several reviews. He has pioneered the development of both coherent multidimensional spectroscopy

methods, associated ultrafast laser technology, and introduced the concept of using ultrabright electron sources to probe structural dynamics. The electron sources developed by his group are sufficiently bright to literally light up atomic motions in real time. He and his group were the first to capture atomic motions during the defining moments of chemistry - to directly observe the very essence of chemistry. This work accomplished one of the dream experiments in science, to bring the chemists? collective gedanken experiment of chemistry to direct observation.

His research accomplishments have been recognized with an A.P. Sloan Fellowship, Camille and Henry Dreyfus Teacher-Scholar Award, Guggenheim Fellowship, Presidential Young Investigator Award (USA), Polanyi Award, Rutherford Medal in Chemistry, the Chemical Institute of Canada (CIC) Medal, and numerous named lectureships. He was inducted as a Fellow of the Royal Society of Canada, Fellow of the CIC, Fellow of the Optical Society of America, and distinguished University Professor at the University of Toronto. He recently received the E. Bright Wilson Award in Spectroscopy, conferred by the American Chemical Society (2015), the Centenary Prize from the Royal Society of Chemistry (2016), and Doctorate of Science Degree (honoris causa) from the University of Waterloo (2017). He is also a strong advocate for science promotion. He earned the McNeil Medal from the Royal Society of Canada (2011) for founding Science Rendezvous, the largest celebration of science (geographically at least) with over 300 events all across Canada, with new initiatives in the North, aimed to make science accessible to the general public.

One of the dream experiments in science has been to watch atomic motions on the primary timescales of chemistry. This prospect would provide a direct observation of the reaction forces, the very essence of chemistry, and the central unifying concept of transition states that links chemistry to biology. This experiment has been referred to as i¿½making t e molecular moviei¿½ with respect to observing net rms atomic motions during struct ral changes. There are not only extraordinary requirements for simultaneous spatial-temp ral resolution but equally important, due to sample limitations, also one on source brightne s. Taking the problem to be an imaging problem, as one makes the shutter speed shorter and shorter, a brighter and brighter source is needed to maintain image contrast. With the development of ultrabright electron capable of literally lighting up atomic motions, his experiment was first realized (Siwick et al Science 2003) and efforts accelerated with the onset of XFELs (Miller, Science 2014). A number of different chemical reactions wil be discussed from electrocyclization with conserved stereochemistry (Jean-Ruel et al J P B 2013), intermolecular electron transfer for organic systems (Gao et al Nature 2013; Liu e al Chem Phys Lett 2017), metal to metal electron transfer (Ishikawa et al, Science 2015), to the recent observation of coherently directed bond formation using the classic I3- system, n a process analogous to a quantum Newton?s cradle (Xian et al Nature Chem 2017). T

ese studies have discovered that these nominally 100+ dimensional problems, representing
the number of degrees of freedom in the system, distilled down to atomic projections alo
g a few principle reaction coordinates. The specific details depend on the spatial resolutio
 to these motions. The most dramatic example will be shown for the simplest form of chemis
ry, electron transfer, which is the heart of redox chemistry. No bonds are made or broken.
The reaction coordinate is dictated by medium repolarization that stabilizes the charge tran
fer state. This motion was captured with sub-A (.01 A) and 100 fs timescale resolution (Ishak
wa, Hayes et al Science 2015) - the fundamental space-time resolution to following the pri
ary processes of chemistry. Without any detailed analysis, the key large-amplitude modes
can be identified by eye from the molecular movie. This reduction in dimensionality appears t
 be general, arising from the very strong anharmonicity of the many body potential in the bar
ier crossing region. We now are beginning to see the underlying physics for the general
zed reaction mechanisms that have been empirically discovered over time. The "magi
 of chemistry" is this enormous reduction in dimensionality in the barrier crossing region
hat ultimately makes chemical concepts transferrable. How far can this reductionist vie
 be extended with respect to complexity? The ultimate goal in scaling system complexity i
 to obtain atomically resolved protein functions to understand how nature tamed chemistry
ver all conceivable length scales. New approaches based on the prinicples used for femtose
ond electron diffraction, both in terms of source technology and image reconstruction,
old promise for real space studies of single biomolecules. This prospect is within reach and
ill provide a definitive test of the collective mode coupling model (Miller Acc. Chem. Rese
rch 1994) to bridge chemistry to biology, which will be discussed as the driving force for
his work.

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