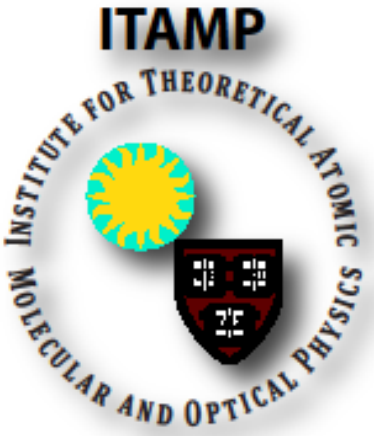
Joint Quantum Sciences Seminar (in Chemistry)



Harvard Department of
Chemistry & Chemical Biology

Prof. Nimrod Moiseyev

Technion - Israel Institute of Technology

Wednesday, May 4, 11:00 am

Pfizer Auditorium Hall | 12 Oxford Mallinckrodt B23

"Non-Hermitian Quantum Mechanics (NHQM) theory for cold molecular collisions"

In this talk I will described briefly the cold collision experiments conducted in Weizmann that motivated this work. Then I will describe the need for NHQM to study the dynamics in scattering experiments in which electrons and the nuclei motion are strongly coupled. In particular I will describe how NHQM enables us to use the Born Oppenheimer approximation for ionizing states that are embedded in the continuum part of the electronic spectra. A new ab-initio method will be presented that enables us the use of standard electronic molecular structure packages for calculating complex potential energy surfaces (CPES). These CPES are used for calculating the cross sections for cold collisions of an excited He (in a triplet spin state) with a (para/ortho) Hydrogen molecule. The products are He in its ground singlet electronic state, molecular hydrogen cation and a free electron. The agreement of our results (obtained from ab-initio non-perturbative calculations) with experiment is remarkable.

Quantum Sciences Seminars (in Chemistry) are jointly sponsored with Harvard Department of Chemistry and Chemical Biology and the Harvard-Smithsonian Center for Astrophysics. ITAMP sponsors talks and presentations on forefront AMO/Condensed Matter Physics from notable Scientists, Researchers and Professors. Information about speakers and ongoing dates can be found on the ITAMP Google Calendar. Go to: http://www.cfa.harvard.edu/itamp/gcalendar.html

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