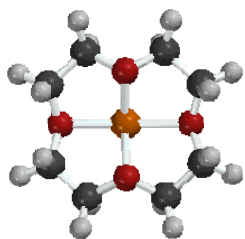


## AMOP Seminar

# *Electron Collisions with Li<sub>2</sub>: the Molecular R-Matrix Method*

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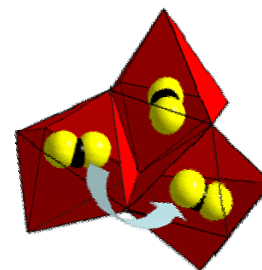
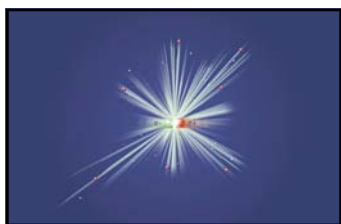


The electron scattering off the lithium dimer represents a challenge for quantum scattering theory methods. Li<sub>2</sub> is a weakly bound molecule with an equilibrium internuclear separation of 5.05 Bohr and a dissociation energy of about 1 eV. The very large bond length leads to a large static dipole polarizability which is among the largest known for molecules.

Quite extensive theoretical and experimental attention has been paid to the structure of the Li<sub>2</sub> molecule as well as to the structure of its negative ion. In contrast, only very few publications concerning the electron scattering off Li<sub>2</sub> are available. All the ab initio calculations of the electron scattering available show an uncertainty for energies below 1 eV or strong dependence on the representation of the target.

The present work investigates low-energy electron scattering off Li<sub>2</sub> in the fixed-nuclei approximation using the R-matrix theory. It is well known that a large polarizability of a target complicates the convergence in calculations based on the close-coupling expansion of the N+1 particle wave function. We focus our attention on the representation of the target giving the correct static dipole polarizability as well as on the long-range effects of the polarization potential outside the R-matrix sphere using the R-matrix propagation. In addition, we discuss the existence of a stable negative ionic state as a function of the internuclear distance. The work presented is the first part of a larger project dealing with Li<sub>2</sub> leading

to calculations of non-elastic processes like vibrational excitation and dissociative electron attachment.



**Wednesday, 19 November 2008**

Brace Lab 202, 3:30pm