Electron-Impact Vibrational Excitation of Molecular Hydrogen

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Electron-impact vibrational excitation of molecular hydrogen in the ground electronic state is one of the most fundamental processes in electron-molecule scattering. The production of vibrationally-excited H2 is of importance in modelling hydrogenic plasmas, as the cross sections for electronic excitation and dissociative processes have a strong dependence on the initial vibrational level [1,2].

Above the threshold for excitation of the electronic singlet manifold, the dominant mechanism for exciting vibrational levels in the ground electronic state is electronic excitation followed by radiative cascade. Calculations of these processes require a fully vibrationally resolved description of the scattering problem, with an accurate account of electronic channel coupling over a large range of internuclear separations. Previous calculations are limited to those performed using the semi-classical impact-parameter method [3], which is known to yield cross sections up to two times larger than convergent close-coupling (CCC) results for electronic excitation [4]. Using a spheroidal-coordinate formulation of the molecular CCC method, we have performed fully quantum-mechanical calculations of excitation-radiative decay (ERD) leading to vibrational excitation of H2, over the range of energies from 10 to 300 eV.

At lower energies, direct vibrational excitation is the only mechanism for producing vibrationally excited H_2. There has been a long-standing interest in theoretical calculations of the $v = 0 - 1$ excitation due to the disagreement between the two principle experimental methods (crossed beam and swarm analysis). In the energy region of interest, the assumptions of the often-used adiabatic approximation for separating the nuclear and electronic degrees of freedom become invalid, and it is necessary to properly account for the coupling between vibrational levels. Vibrational close-coupling (VCC) calculations have been previously performed [5] with the use of polarisation potentials to allow for an approximate treatment of the coupling to electronic excitations. In this talk we will review the existing calculations and experimental results, discuss the more accurate account of target polarisation possible with the CCC method, and present new VCC results for the direct vibrational excitation of H_2 by low-energy electrons.

References
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