Charge Transfer Cross sections Calculation for O^{6+}-H Collisions

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Synopsis The full quantum-mechanical molecular orbital close-coupling (QMOCC) methods is employed to study the charge transfer process in collisions of O^{6+}-H in the energy region from 10^{-3}keV/u to 6keV/u. Total and state-selective cross sections obtained are in good agreements with the available experimental data. In combination with the two-center atomic orbital close-coupling (TC-AOCC) method calculations, the converge on the reaction channels number in the QMOCC calculations are demonstrated for total and the dominant state-selective cross sections of *4l*.

The charge transfer in collisions of O^{6+}+H is one important highly charged ions collisions processes in the solar wind X-ray studies. In the present work, the total and state-selective charge transfer cross sections are calculated by using QMOCC method [1] in energy region 10^{-5}-6keV/u. The *ab initio* multi-reference single and double excitation configuration interaction (MRD-CI) method [2-3] is employed to calculate the radial and rotational coupling matrix elements used in the QMOCC calculations.

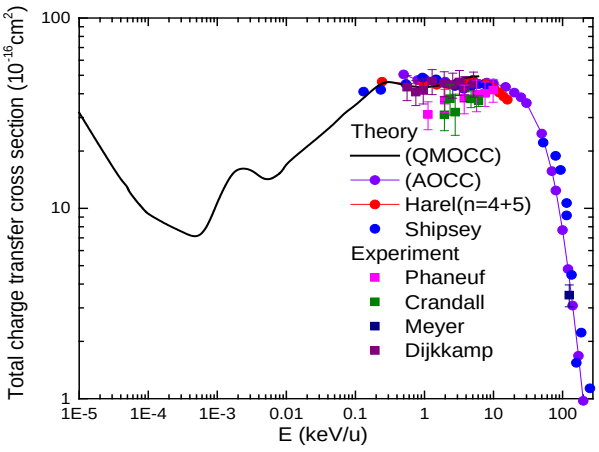

Figure 1. Total charge transfer cross sections for the O^{6+}-H(1s) collisions as a function of the cereollision energy. Theory: (—) AOCC results; (—) results of Harel *et al* [7]; (▲) results of Shipsey *et al* [6]. Experiment: (◆) Crandall *et al* [5]; (★) Dijkkamp *et al* [4]; (■) Meyer *et al* [8]; (●) Phaneuf *et al* [9]

As shown in Fig.1, the present calculations are compared with the available theoretical and experimental results [4-9]. Note that the excited states of O^{5+} (*n l*) are included up to n=6 in the QMOCC calculations to obtained converged results. From Fig.1, it can be observed that the present MOCC calculations are in better agreement with the measurement of Dijkkamp *el al* [4], Crandall *el al* [5] and Phaneuf *el al* [9] in comparison with other calculations [4, 6-8] in the overlapped energy range.

In order to check the convergence on the channels number included in the close-coupling calculation, the AOCC calculations are also performed with inclusion of different excited state channels of O^{5+} (*n l*; n=5, 6 and 9) respectively in the energy range of 1-5keV/u. It is found that the contributions from higher excited states of n > 6 are less than 5%. Furthermore, the contributions from excited states of H(*n l*) are also found to be negligible.

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