Hyperspherical close-coupling calculations for charge transfer in Si^{4+}+H, Be^{4+}+H, H^++Na and H^++D collisions

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We have used the recently developed hyperspherical close-coupling (HSCC) method for ion-atom collisions [1] to calculate charge transfer cross sections for a number of collision systems at low energies (below a few keV/amu) . In the HSCC method, we model each collision system as consisting of one electron in the Coulomb field (or a model potential) of the two nuclei (or two cores) and solve the resulting Schrödinger equation in hyperspherical coordinates. The wavefunction is first expanded in terms of adiabatic channel functions with the hyperradius treated as the adiabatic parameter and the resulting hyperradial wavefunction is solved using the R-matrix propagation method. Here we report the HSCC results for some collision systems:

(1) Si^{4+}+H(D)

The total charge transfer cross sections for this system has been studied experimentally [2] for energies between 0.01 to 1000 eV/amu. The HSCC results are in agreement with calculations based on the molecular orbital expansion method where the translational effect is accounted for by the use of reaction coordinates (RC). The cross section ratios for capture to 3d and to 4s were found to disagree with the experiment of Wu and Havener [3] but in agreement with the molecular calculations reported in [2]. The isotope effect has been observed at low collision energies for this system.

(2) Be^{4+}+H

The total electron capture cross sections for this system for v below 0.2 a.u. have been calculated and the results compared well with the calculations using the reaction coordinate method of Errea et al [4]. For the partial wave cross sections we observed that there are discrepancies at low energies. The cross sections for capture to the weaker n=4 manifold also show some differences at low energies.

(3) H^+ +Na

We have examined this collision system in view of the existing discrepancies in the literature. The total charge transfer cross sections calculated by Dutta et al [5] are in good agreement with experiment but in disagreement with the RC calculations of Croft and Dickinson [6]. Our results agree with the latter except for energies below 3 eV.

(4) Excitation and charge transfer to 2p states in H^++H(D)

For H^++H collisions below 1 keV, besides the resonant charge transfer procecss, the only important inelastic processes are excitation and charge transfer to the 2p state by rotational coupling. We used the HSCC method to obtain these cross sections from the threshold to 2keV in view of such cross sections are not available in the literature in the low energy region.

References

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