# § 8. Molecular Orbital Study Ionization in Low-Energy $He^{2+}$+H(1s) AND $He^{+}$(1s)+$H^{+}$ Collisions

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The one-electron $HeH^{2+}$ system is a prototype for investigating heteronuclear collision systems, for which a numerous works have been done on both theoretical and experimental sides. Yet, most of these works are focus on exciation/capture process, ionization is left to be understand and remains a challenge. Accurate ionization cross sections of $He^{2+}$+H and/or $He^{+}$+$H^{+}$ collision systems, however, are essential important for plasma diagnostics in fusion devices.

To address the issue of ionization, we have employed the close-coupling method with $HeH^{2+}$ molecular states as basis and electron translation-factor corrections based on molecular-state switching functions, to compute the total and differential ionization cross sections for (a) $He^{2+}$+H(1s) and for (b) $He^{+}$(1s)+$H^{+}$ collision systems at projectile energies 1-20 keV/amu. Basis sets with up to 20 bound states and 12 partial waves at 32 energies for continuum states have been used, and good convergence of results as a function of basis size is found. We should emphasize that the exact wavefunctions of physical continuums are employed in the present calculation without any discretization. The number of continuum state energies mentioned above is the number of interpolation knots for integration. It should be not confused with pseudostate expansion. This approach has been successfully applied to study ionization processes in low-energy proton-hydrogen collisions [1].

The results are compared with recent theoretical calculations and available experimental values [2]. Good agreement is found with recent experimental measurements. Total ionization and state-selected charge transfer cross sections resulting from a $He^{2+}$+H(1s) collision are plotted in Fig. 1 and 2 as part of the preliminary results.

We find the degeneracy of $3d\sigma$ and $2p\sigma$ at $R \to \infty$ plays an important role in the ionization of H(1s) by $He^{2+}$. The $2p\sigma \to 3d\sigma$ excitation caused by long range radial coupling enhance the total ionization cross sections by factors of 4 through 6 in most the energies considered above. Hence, it appears that the "ladder-climbing" process is the most important ionization mechanism in $He^{2+}$+H(1s) collisions.

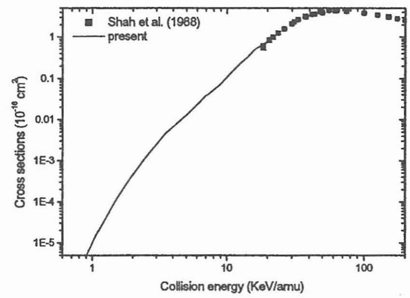


Fig. 1. Total ionization cross sections resulting from a $He^{2+}$+H(1s) collision.

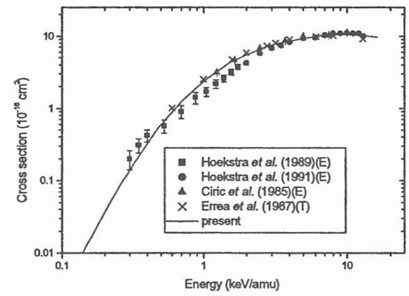


Fig. 1. Charge transfer cross sections of $He^{2+}$+H(1s)$\to He^{+}(n=2)$+$H^{+}$ at low energies.

## References

[1] S. Zou, L. Pichl, M. Kimura and T. Kato, Phys. Rev. A. **66**, 042707(2002).

[2] M.B. Shah, and D. S. Elliot, P. McCallin, and H. B. Gilbody, J. Phys. B. **21**, 2455(1988).