Model for vibronic excitation of CH^+ by resonant scattering of electron

Model for vibronic excitation of CH^+ by resonant scattering of electron

X Jiang[1], C Yuen[2], P Cortona[1], V Kokoouline[2] and M Ayouz[3] *

[1] SPMS, CentraleSupélec, Université Paris-Saclay, 91190, Gif-sur-Yvette, France
[2] Department of Physics, University of Central Florida, 32816, Florida, USA
[3] LGPM, CentraleSupélec, Université Paris-Saclay, 91190, Gif-sur-Yvette, France

Synopsis A new model for theoretical study of vibronic (de-)excitation (including vibrational (de-)excitation) cross sections of CH^+ by electron impact was developed based on the multichannel quantum defect theory (MQDT) close-channel-elimination procedure and vibrational-frame-transformation theory of Chang and Fano. The successful application of this model suggested a promising calculation method for vibronic (de-)excitation of diatomic ion core by resonant scattering of electron.

Vibrational-frame-transformation theory of Chang and Fano [1] is extensively used to describe the vibrational (de-)excitation of nonresonant electron molecule (ions) collision system. Fixed-nuclei R-matrix method is perfectly combined with this theory to provide a smooth short-range scattering matrix (S-matrix) in the Body frame (BF) [2, 3]. However, difficulties emerged for this theory to understand the vibrational excitation for the e-CH^+ collision system of great astrophysical and technological plasma interest. This was ascribed to the strong energy dependence of the short-range S-matrix for the collisions. Meanwhile, the non-adiabatic method coupling with vibrational motion of the nuclei for this collision system would be extremely time-consuming due to the low-lying electronically excited states of CH^+. Accordingly, this process was far from being precisely modeled in theory.

In this study, we propose a new model based on the MQDT close-channel-elimination procedure and the vibrational-frame-transformation theory to compute vibronic (de-)excitation cross sections and thermally-averaged rate coefficients for e-CH^+ collisions. In this model, the R-matrix formalism is employed to evaluate the electron-ion S-matrix in BF frame for a fixed geometry of the ion core. The electron scattering energy was extended to a highly excited state level where the S-matrix with multiple open electronic excitation channels is smooth. The S-matrix describing the vibronic transition is obtained from the vibronic-frame-transformation and MQDT close-channel-elimination procedure. The electronic excitation cross sections obtained in this model was compared with that from UKRmol suite [4], which was shown in Figure 1. A well matched behavior suggested the validation of our model. Finally, fitting formulas with a few numerical parameters were derived for the obtained rate coefficients. The interval of applicability of the formulas is from 40 to 10,000 K.

This model that has been applied successfully to the e-CH^+ system provides a potentially unified theoretical treatment for the vibronic (de-)excitation of other diatomic molecular ions by resonant scattering of electron. Further attempts will be taken to generalize this model to those collisions of polyatomic molecular ions and electrons.

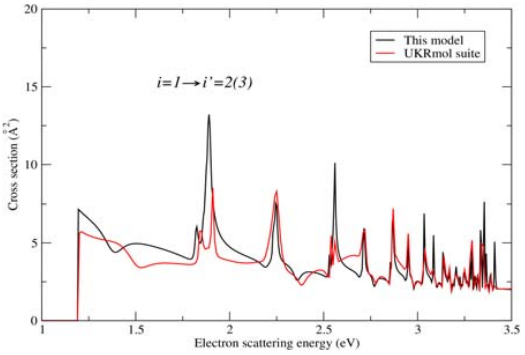

Figure 1. The comparison of the electronic excitation cross section for $X^1\Sigma^+$ (i=1)-$a^3\Pi$ (i=2(3)) at equilibrium nuclear distance (R=2.137 bohr).

References

[1] Chang E S, Fano U 1972 *Phys. Rev. A*. **6** 173
[2] Ayouz M, Kokoouline V 2016 *Atoms*. **4** 30
[3] Aymar M *et al* 1996 *Rev. Mod. Phys.* **68** 1015
[4] Tennyson J *et al* 2007 *J. Phys. : Conf. Ser.* **86** 012001

* E-mail: mehdi.ayouz@centralesupelec.fr