Ab initio study of proton collisions with BeH

I. Rabadán [*1], L.Méndez [*], J. W. Gao [†‡], Y. Wu [†], J. G. Wang [†]

[*] Departamento de Química, Universidad Autónoma de Madrid, 28049 Madrid, Spain
[†] Institute of Applied Physics and Computational Mathematics, 10088 Beijing, China
[‡] Laboratoire de Chimie Physique Matière et Rayonnement, UMR 7614, UPMC Univeristé Paris 6, Paris, France

Synopsis We present calculations of electron capture cross sections in proton collisions with BeH molecules in the energy range 25 eV/u $< E <$25 keV/u.

A key issue in the design of future fusion tokamaks is the choice of plasma facing materials. In ITER, beryllium will be the plasma facing component of the main chamber. An ITER-like-wall is currently installed in the Joint European Torus (JET) and several experiments have already been carried out in order to understand the erosion of the first wall and the material migration. Some of these experiments [1] have pointed out the importance of the chemical assisted physical sputtering mechanism that leads to the release of BeD molecules, which are then ionized and dissociated by collision with the main plasma components.

In this work, we present a theoretical study of the electron capture (EC) reaction

$$H^+ + BeH(^2\Sigma^+) \rightarrow H + BeH^+ \qquad (1)$$

Orientation-averaged total cross sections are obtained by expanding the scattering wave function in a basis set of molecular electronic states of the H_2Be^+ molecule. Our treatment assumes rectilinear projectile trajectories and uses the sudden approximation for molecular rotation and vibration. The molecular wave functions have been obtained with a 3-electron full configuration interaction (CI) method, with the 1s electrons of Be frozen. As an illustration, we show in Fig. 1 a cut of the potential energy surfaces (lines) for a nuclear geometry in which the BeH target is fixed at the equilibrium distance of its electronic ground state ($\rho_e = 2.568$ bohr). One can note the good agreement with the energies calculated with a multi-reference single- and double-excitation CI method [2] (solid symbols).

We show in Fig. 2 the orientation-averaged EC cross sections calculated within the Franck-Condon approximation ($\rho = \rho_e$). Here, we note that the transitions to the EC channels that dissociate into $H(1s)+BeH^+(2^1\Sigma^+,1^3\Pi)$ (3-state calculation), furnish the main mechanism of reaction (1). The importance of including rotational couplings, and not only radial ones, in the calculation is also emphasized in the figure. In addition, SC-AOCC calculations [3] will also be performed for higher energies in the future. The relatively large cross section for this reaction indicates that it could be relevant in plasma modelling.

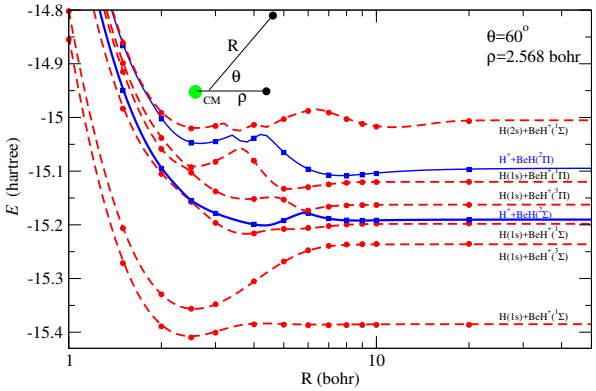

Figure 1. Potential energy curves of H_2Be^+ for the nuclear geometry shown in the figure.

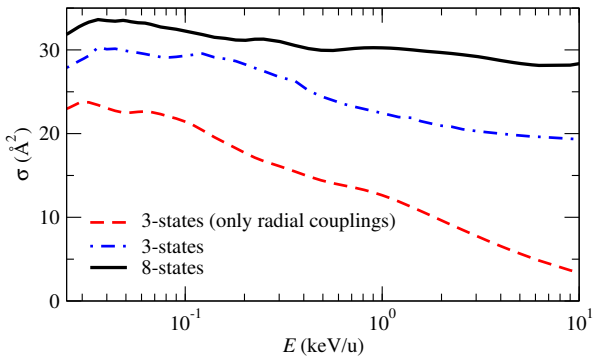

Figure 2. Orientation-averaged EC total cross section for reaction (1) as a function of the collision energy.

This work has been partially supported by a project UAM-Santander de Cooperación Interuniversitaria con Asia and Ministerio de Economía y Competitividad (Spain) (ENE2014-52432-R).

References

[1] S. Brezinsek *et al.* 2015 *Nuclear Fusion* **55** 063021

[2] R. J. Buenker and R. A. Phillips 1985 *J. Mol. Struct. THEOCHEM* **123** 291

[3] N. Sisourat *et al.* 2011 *Phys. Rev. A* **84**, 052722

[1] E-mail: ismanuel.rabadan@uam.es