Contribution ID: **343** Type: **Oral Presentation**

Theoretical studies of mutual neutralization in collisions of He⁺ + H[–] and Li⁺ + F[–].

Thursday, 2 July 2015 16:50 (20 minutes)

Abstract content
   (Max 300 words)
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Employing electronic structure techniques with the full configuration interaction (FCI) method, potential energy curves of the electronic states relevant in mutual neutralization of He⁺ + H[–] collisions are calculated. We also compute the non-adiabatic couplings between the states. To complement this calculation, at short internuclear distances, electron scattering calculations, based on the complex-Kohn variational method is employed to compute energy positions and autoinisation widths of the resonant states.

Employing a complete-active-space self-consistent field (CASSCF) method, potential energy curves of the states relevant for low energy (0-100 eV) mutual neutralization collisions of Li⁺ + F[–] are computed. Here a set of eight basis sets is used to obtain the states and their corresponding non-adiabatic couplings.

The non-adiabatic couplings vary rapidly with internuclear distance and may cause numerical challenges. It is common practice to transform the potential energy from an adiabatic representation to a diabatic representation. A strict diabatazition is performed, to obtain the potential energy curves of diabatic states that are crossing each other.

The nuclear dynamics are studied with the diabatic representation, using Johnson's log derivative method. We report the total and differential cross sections of the neutralization reactions. The final states distributions are also calculated. We also investigate the influence of autoinisation on the reaction as well as isotope effect. The results are compared with experimental data.

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Main supervisor (name and email)
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Session Classification: TCP

Track Classification: Track G - Theoretical and Computational Physics