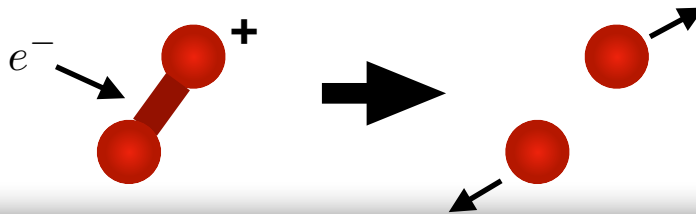


Dissociative Recombination with a Scattering Matrix Approach; HeH⁺ as a Test Case

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Dissociative Recombination (DR):



The method uses a computationally inexpensive approach to obtain the DR cross section [1] and Quantemol's QN software [2] to run R-matrix calculations.

Calculations can be run at low computational expense with very good correlation between this method and a more full calculation of the diatomic HeH⁺ [3] at low energy.

The only outliers between the methods are resonances that are accounted for in the previous more rigorous expensive calculation, as shown in the below graph.

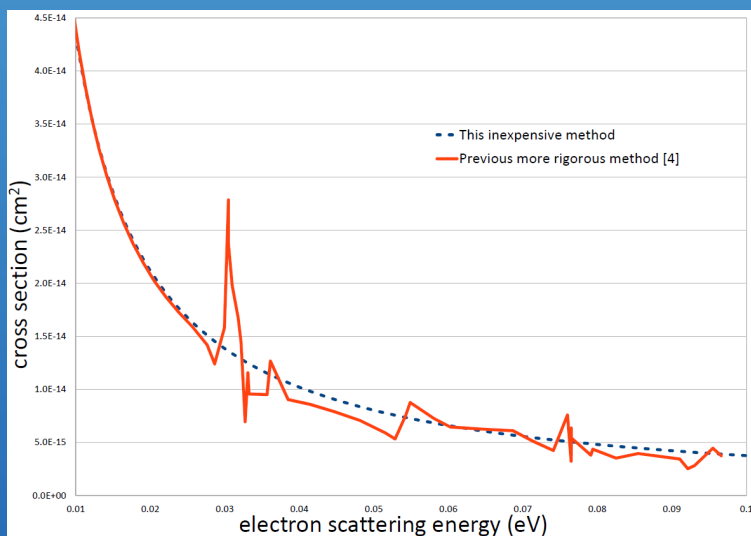


Figure 1: Graph comparing the current inexpensive method of calculating DR cross sections using the equation below (dashed line) and the previous more rigorous method [3] (solid line).

$$\langle \sigma \rangle = \frac{\pi \hbar^2}{4m\epsilon} \sum_{i=1}^{3N-5} \sum_{l'l'\lambda\lambda'} \left| \frac{\partial S_{l\lambda, l'\lambda'}}{\partial q_i} \right|$$

In this method of calculating the DR cross section [1]:

- the rotation of the molecular target is neglected,
- the cross section is averaged over autoionizing resonances,
- autoionization lifetime is assumed to be much longer than the predissociation lifetime,
- the harmonic approximation is used to describe the vibrational states of the core ion.

By taking small changes in molecular geometries, you can get an estimate of the cross section using this method.

The cross section for each collision energy, is a function of the sum over all channels of the change in the S-Matrix element over the change in geometry (i.e. small change in internuclear distance from equilibrium).

The plan is to apply this methodology to polyatomic systems which are yet amenable to a full treatment.

References:

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