Modeling ultracold lithium ion-atom collision

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Synopsis Accurate estimation of the scattering properties at the ultracold temperatures is challenging due to the demand for the precise knowledge of interactions between the colliding partners. We identify the aspects of interactions that play the defining roles in the scattering calculations. We compute potential energy curves for the $^7Li^+$-^7Li, $X^2\Sigma_g^+$ and $A^2\Sigma_u^+$, and determine their collisional properties.

In the study of the ion-atom interactions at ultracold temperatures, Li^+-Li is one of the most advantageous candidates for attaining the *s*-wave and few partial wave regime for their mutual scattering. This is because of the combination of its reduced mass and polarizability [1,2].

Scattering processes in the $^7Li^+$-^7Li ion-atom system for temperatures starting from a few K to sub-μK are investigated. Accurate potential energy curves (PECs) of the ground and first excited state of the Li_2^+ molecular ion, $X^2\Sigma_g^+$ and $A^2\Sigma_u^+$, are calculated, (Fig. 1), in order to estimate the low energy scattering phase shifts, which are employed to compute the ion-atom total scattering cross section for the system. The PECs are computed using the multi-reference configuration interaction (MRCI) method with Dunning correlation-consistent polarized, core-valence, augmented, 5-zeta, (aug-cc-pCV5Z), basis sets in the range of internuclear separations 2-50 atomic units. Numerical extrapolations to generate the PECs outside this range are performed.

We discuss the contributions arising from the $X^2\Sigma_g^+$ and $A^2\Sigma_u^+$ states for both scenarios when the identities of the participating entities, Li^+ and Li, are retained or interchanged in the collision events. These two collision channels can be described only in the high energy limit as direct elastic and resonant charge exchange (RCE) collisions [3]. At very low energies, it is impossible to assign the outcome of the collision to one or other of these channels. Results of the cross section calculations will be presented at the conference.

In addition, we examine the effects of minor alterations in small-R regions of the calculated PECs, where the ab-initio molecular calculations can have significant uncertainties, on the scattering parameters. We find that in the *s*-wave limit, the cross section terms involving $X^2\Sigma_g^+$ state is sensitive to the minor alterations in the PEC; the effect is amplified as the low energy scattering is close to a pole. We provide a comparison of the properties of PECs and scattering parameters with previous experimental and theoretical results and review the essential elements for reliable estimation of the collision cross sections [4].

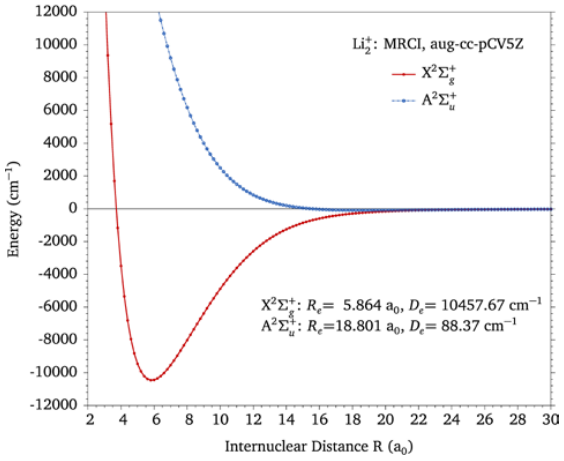

Figure 1. The first two states of Li_2^+, $X^2\Sigma_g^+$ and $A^2\Sigma_u^+$, computed using the MRCI method with aug-cc-pCV5Z basis set are shown.

References

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