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Non-Adiabatic Quantum Dynamics of the Ultracold Li+LiNa→ Li₂+Na Chemical Reaction

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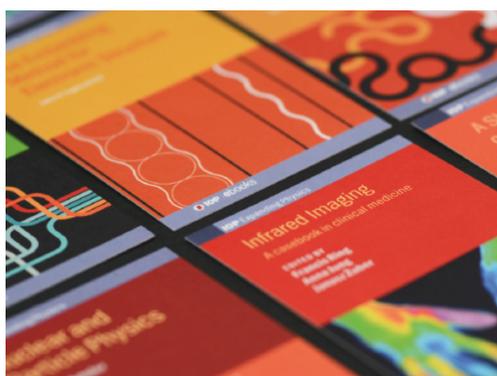
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Non-adiabatic quantum dynamics of the ultracold $\text{Li}+\text{LiNa} \rightarrow \text{Li}_2+\text{Na}$ chemical reaction

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Synopsis We report non-adiabatic dynamics of the $\text{Li}+\text{LiNa} \rightarrow \text{Li}_2+\text{Na}$ chemical reaction at cold and ultracold temperatures employing accurate ab initio electronic potential energy surfaces in a quantum dynamics formulation employing a diabatic representation. Results are compared against those from a single adiabatic ground state potential energy surface and a universal model based on the long-range interaction potential. We discuss signatures of non-universal behavior in the total rate coefficients as well as strong non-adiabatic effects in the state-to-state rotationally resolved rate coefficients.

Ultracold molecules, polar molecules in particular, are now at the forefront of precision spectroscopy, sensing, controlled studies of chemical reactions, quantum many-body physics, and quantum computing. Polar molecules comprised of heteronuclear alkali metal dimers such as KRb, NaK and LiNa have attracted considerable attention in recent years in controlled studies of chemical reactions. Electronically non-adiabatic effects are expected to play an important role in atom-dimer reactions involving these systems, e.g., $\text{K}+\text{KRb}$ or $\text{Li}+\text{LiNa}$. These systems exhibit a conical intersection (CI) between the ground electronic state and the first excited doublet electronic state. The CI becomes accessible even for collision energies in the ultracold limit for ground state reactants. Explicit quantum calculations for these reactions remain a formidable challenge even for dynamics on a single adiabatic electronic potential surface.

Here, we report a first principles quantum dynamics study of non-adiabatic effects in $\text{Li}+\text{LiNa}(v=0, j=0) \rightarrow \text{Li}_2(v', j')+\text{Na}$ reaction and compare results against a calculation that neglects non-adiabatic and geometric phase effects as well as that obtained using a universal model based on long-range forces. Details of the quantum dynamics method are given elsewhere [1]. Figure 1 compares non-thermal rate coefficients for total angular momentum quantum number $J=0$ (s-wave scattering in the incident channel) from the two-state calculations

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within a diabatic representation against a single surface calculation that excludes any geometric phase and non-adiabatic effects. The results correspond to even exchange symmetry (exchange of the two identical Li atoms). It is seen that the limiting values of the total and vibrationally resolved rate coefficients differ by factors of about 1.2 and 1.6. For rotational resolved rates, the results differ by an order of magnitude or more between 2-state and single surface calculations.

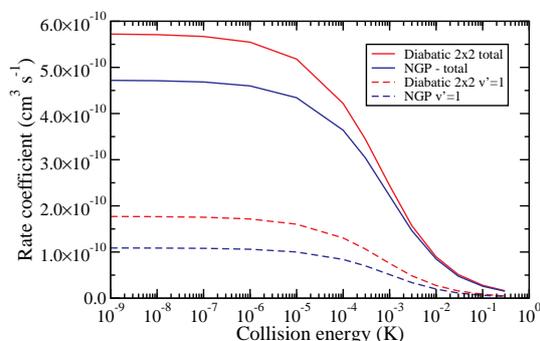


Figure 1. Rate coefficients for the $\text{Li}+\text{LiNa}(v=0, j=0) \rightarrow \text{Li}_2(v')+\text{Na}$ reaction as a function of the collision energy. The diabatic 2×2 results correspond to the two-state calculation that implicitly accounts for the geometric phase effect. The NGP (no-geometric phase) result corresponds to a single ground state adiabatic potential. The results are for even exchange symmetry of the identical Li atoms and do not include nuclear spin-statistics factors.

References

- [1] Kendrick B K 2018 *J. Phys. Chem.* **148** 044116

