Magnetic tuning of ultracold chemical reactions: Theoretical insights

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Attaining external field control of bimolecular chemical reactions has long been a coveted goal of physics and chemistry. To explore how hyperfine interactions and magnetic fields can be used to achieve such control, we develop an extended coupled-channel statistical theory of barrierless atom-diatom chemical reactions, and apply it to the chemical reaction $\mathrm{Li}(^2\mathrm{S}_{1/2}) + \mathrm{CaH}(^2\Sigma^+) \rightarrow \mathrm{LiH}(^1\Sigma^+) + \mathrm{Ca}(^1\mathrm{S}_0)$ on a newly developed set of *ab initio* potential energy surfaces. We observe large field effects on the reaction cross sections, opening up the possibility of controlling ultracold barrierless chemical reactions by tuning selected hyperfine states of the reactants with an external magnetic field [1].
We also propose a new statistical approach to address the two central problems in ultracold molecular collision theory: (1) slow basis set convergence of molecular scattering observables and (2) their extreme sensitivity to the potential energy surfaces (PESs) underlying quantum scattering calculations. Specifically, we show that the probability distributions that an observable is in a certain range of values can be obtained by averaging the results of scattering calculations with much smaller basis sets than required for calculations of individual scattering cross sections. Moreover, we show that such distributions do not rely on the precise knowledge of the PES, making it possible to probabilistically predict experimentally relevant observables for a wide variety of molecular systems, currently considered out of reach of quantum dynamics theory [2].

References

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