Ultracold highly polar KAg and CsAg molecules: electronic structure and optical formation

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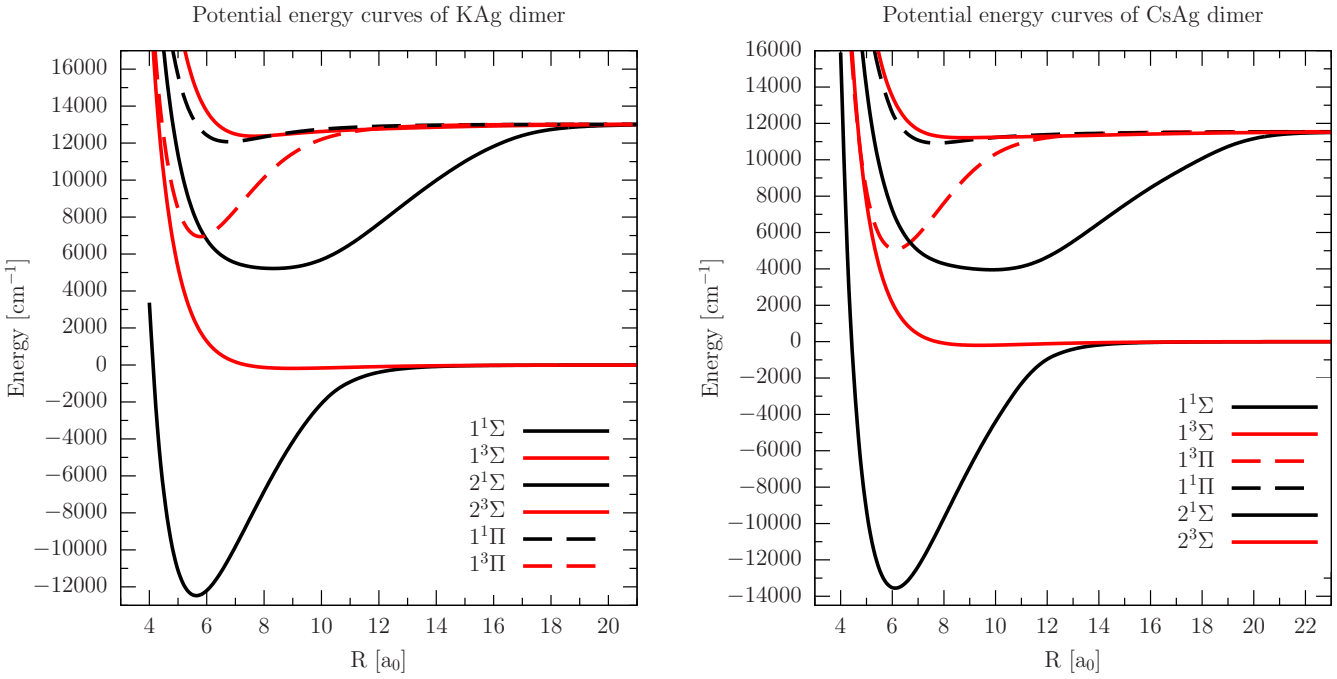
Diatomic molecules consisting of silver and alkali-metal atoms are predicted to possess very large permanent electric dipole moments, approaching 10 debye [1]. In this study, we theoretically investigate the prospects for the formation of ultracold, highly polar KAg and CsAg molecules from ultracold atomic mixtures using photoassociation or magnetoassociation techniques followed by optical stabilization. We calculate the potential energy curves for the first two lowest $^{1,3}\Sigma$ and lowest $^{1,3}\Pi$ states together with the permanent and transition electric dipole moments for the ground and excited electronic states alongside the permanent and transition electric dipole moments for the ground and excited electronic states, employing coupled cluster and multireference configuration interaction methods with large basis sets. Additionally, we determine spin-orbit couplings between these states.



Using the calculated electronic structure data, we calculate vibrational levels, Franck-Condon factors, Einstein coefficients, and radiative lifetimes. We also explore potential pathways for the Stimulated Raman Adiabatic Passage (STIRAP) to transfer weakly bound Feshbach molecules to the absolute ground state. Finally, we assess the experimental feasibility of our proposed approaches.

References

[1] M. Śmiałkowski, M. Tomza, Phys. Rev. A 103, 022802 (2021).