Formation and control of ultracold ytterbium dimers using optical transitions

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Ground and excited electronic states of the ytterbium dimer (Yb_2) challenge modern electronic structure theory. At the same time, weakly bound Yb_2 were already produced at ultralow temperatures and are the perfect starting point for transferring them to the ground state and applications in precision measurements and quantum-controlled chemistry.

The aim of this study is to theoretically predict the optical spectrum and analyze optical transitions in the ytterbium dimer between the singlet ground state $X^1\Sigma_g^+$ and the excited state $A^1\Sigma_u^+$. These investigations provide valuable insights into spectroscopic interactions and the underlying processes involved in the formation of ultracold quantum gases.

Our group has conducted electronic structure calculations using coupled-cluster theory [CCSD(T)] in conjunction with newly developed correlation-consistent Gaussian basis sets ranging from double- to quintuple-zeta quality (aug-cc-pwCVnZ-PP, n = 2–5). To obtain the vibrational and rotational energy levels, we employed the discrete variable representation (DVR) method, which enables efficient and accurate numerical solutions of the nuclear Schrödinger equation. The resulting vibrational wavefunctions were then used to compute Franck–Condon factors by evaluating wavefunction overlap integrals between the ro-vibrational states of the ground and excited states. The resulting Franck–Condon landscape also supports the identification of favorable transition pathways, which is relevant for coherent population transfer techniques such as Stimulated Raman Adiabatic Passage (STIRAP), particularly in the context of ultracold molecule formation.

Our calculations yielded potential energy curves for both the $X^1\Sigma_g^+$ ground state and the $A^1\Sigma_u^+$ excited state, alongside corresponding sets of ro-vibrational energy levels. Using vibrational wavefunctions derived from DVR, we constructed detailed Franck–Condon factor maps, resolved across a wide range of rotational quantum numbers. These two-dimensional maps illustrate transition strengths for multiple channels, including (v, J) $\rightarrow$ (v, J–1), (v, J), and (v, J+1), providing a comprehensive view of the rotationally resolved transition landscape. In addition, we extended our analysis to include mixed isotopic variants of the ytterbium dimer (e.g., ^{172}Yb–^{174}Yb), accounting for their distinct reduced masses and resulting shifts in vibrational structure. The corresponding Franck–Condon maps revealed notable differences in transition intensities and level spacings, highlighting isotope-specific pathways that could be advantageous for optical state preparation or detection in ultracold experiments.

The obtained results provide valuable insights into the spectroscopy of the ytterbium dimer and the mechanisms of optical transitions. The presented analysis enhances the understanding of ultracold quantum gas formation processes and may contribute to further research in optical metrology and quantum technologies.

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