Prospects for ulracold CsYb molecules: a theoretical structural study

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Mixtures composed of alkali-metal and closed-shell atoms open up the possibility of creating paramagnetic ground-state polar molecules, with applications in quantum simulation and quantum information, precision measurement, tests of fundamental physics, and tuning of collisions and chemical reactions [1]. The ultracold CsYb molecule is proposed to be an attractive candidate for the possibilities mentioned.

To our knowledge, there is only one ab initio calculation for the CsYb molecule in the excited electronic states [2], and some experimental data are valuable for the calculation of the structure of the CsYb molecule [1]. However, this ab initial calculation still suffers from too large differences in the dissociation limit energies, the absence of certain electronic states, etc. These problems prevented them from analyzing any calculations above the asymptote Cs ($6s\ ^2$P) + Yb ($6s^2\ ^1$S).

We present a full configuration interaction of the ground and excited CsYb states, described as a three-valence electron system in the field of effective core potentials including core polarization, and obtain the ground and 10 low-lying excited electronic states of the CsYb molecule in five dissociate limits without spin-orbit coupling. Subsequently, we introduce spin-orbit coupling (SOC) terms as an atomic model certainly valid at large distances, which means that the spin-orbit constants are R-independent in our model, and compare 19 electronic states with ab initio calculation results [2], as shown in Fig.1. We report results for spectroscopic constants, vibrational energies, and Franck-Condon factors. All data obtained will allow prediction of the best STIRAP (Stimulated Raman Adiabatic Path), which is a promising route to the creation of ultracold ground-state $^2\Sigma$ molecules.

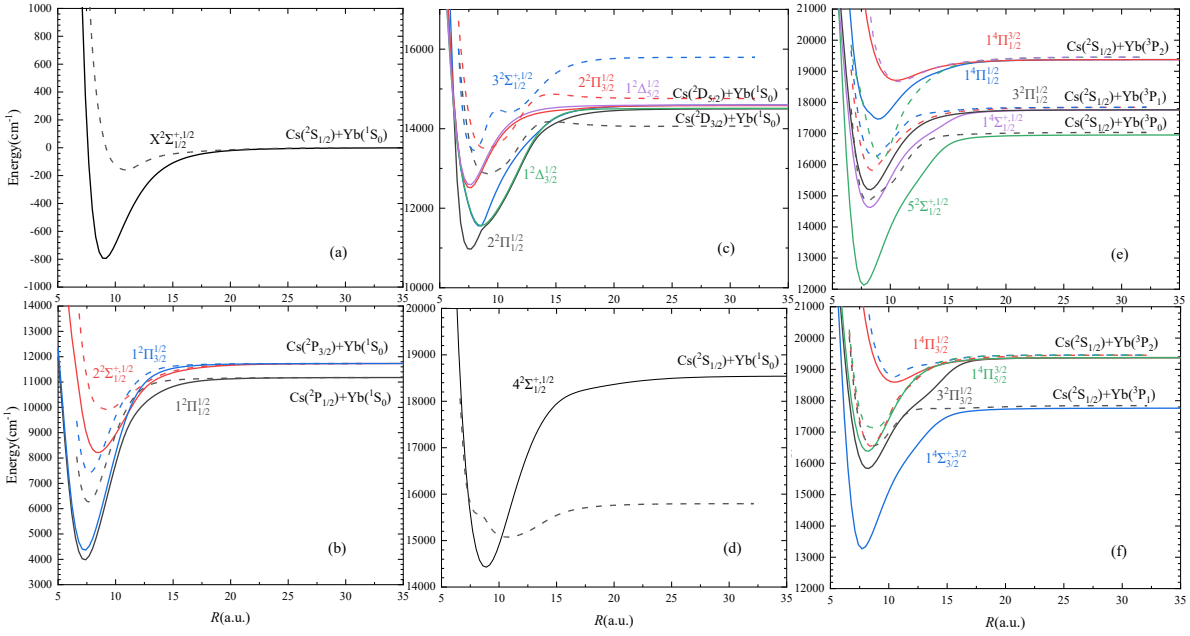

Figure 1: Electric states for CsYb molecule corresponding to the asymptote (a) Cs ($6s\ ^2$S) + Yb ($6s^2\ ^1$S), (b) Cs ($6p\ ^2$P) + Yb ($6s^2\ ^1$S), (c) Cs ($5d\ ^2$D) + Yb ($6s^2\ ^1$S), (d) Cs ($7s\ ^2$S) + Yb ($6s^2\ ^1$S), (e) Cs ($6s\ ^2$S) + Yb ($6s6p\ ^3$P) with $|\Omega| = 1/2$ and (f) Cs ($6s\ ^2$S) + Yb ($6s6p\ ^3$P) with $|\Omega| = 3/2$ or 5/2. Our calculation PECs are shown in solid line and the dash lines are the PECs in Ref.[2]. Within the same subplot, lines in the same color denotes the same electronic state.

References

[1] A. Guttridge, M. D. Frye, B. C. Yang, J. M. Hutson, and S. L. Cornish *Phys. Rev. A* **98** 022707 (2018).
[2] Darya N. Meniailava a, Maksim B. Shundalau,*Computational and Theoretical Chemistry* **1111**, 20–26 (2017).