Full-Range Analytical Potential for the $a^3\Sigma^+$ State of LiNa: Robust Prediction of Vibrational Levels and Scattering Length (Supplemental Material)*

Dongying Li[1] and Xiaowei Sheng[1*]

1. Anhui Province Key Laboratory of Optoelectric Materials Science and Technology, Department of Physics, Anhui Normal University, Anhui, Wuhu 241000, China

*Correspondence

Xiaowei Sheng, E-mail:xwsheng@mail.ahnu.edu.cn

I. COMPARISONS OF $V_{STT}(R)$ WITH THEORETICAL AND EXPERIMENTAL POTENTIAL ENERGY CURVES FOR LIK, LIRB, AND LICS MOLECULES.

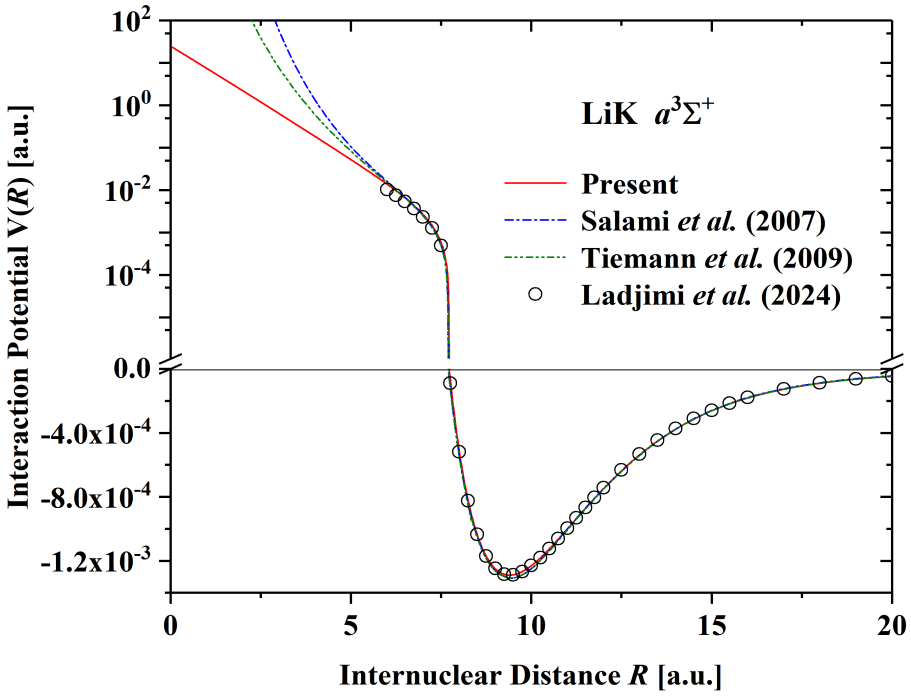

FIG. S1: The potential energy curve for the $a^3\Sigma^+$ state of LiK calculated with the model of STT. The small circles are the *ab initio* results reported by Ladjimi *et al.*[1]. The blue and green lines are the experimental potentials, which are obtained from Ref. [2] and Ref. [3], respectively.

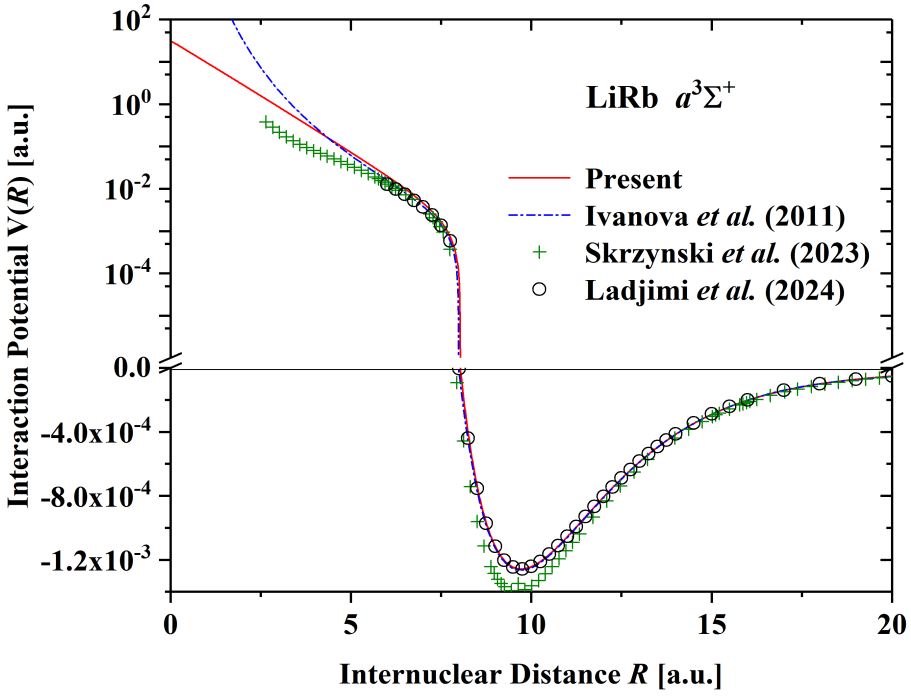

FIG. S2: The potential energy curve for the $a^3\Sigma^+$ state of LiRb calculated with the model of STT. The small circles are the *ab initio* results reported by Ladjimi *et al.*[1]. The blue line is the experimental potential, which is obtained from Ref. [4]. The green points are taken from the supplement material of Ref. [5]

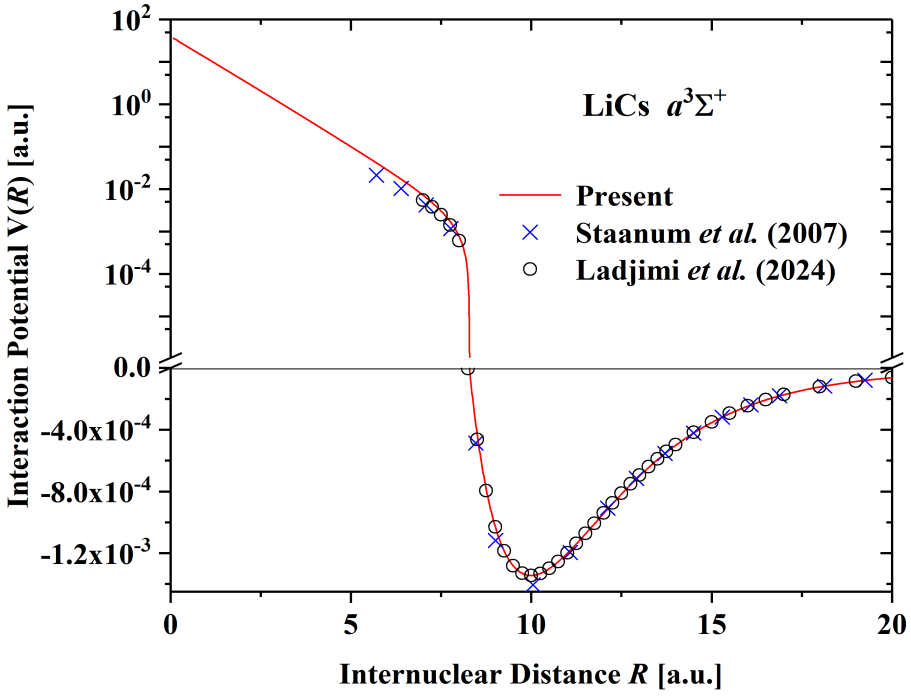

FIG. S3: The potential energy curve for the $a^3\Sigma^+$ state of LiCs calculated with the model of STT. The small circles are the *ab initio* results reported by Ladjimi *et al.*[1]. The blue points are the experimental potential, which are taken from supplement material of Ref. [6].

REFERENCES

[1] H. Ladjimi and M. Tomza, Diatomic molecules of alkali-metal and alkaline-earth-metal atoms: interaction potentials, dipole moments, and polarizabilities, Phys. Rev. A **109**, 052814 (2024).

[2] H. Salami, A. J. Ross, P. Crozet, W. Jastrzebski, P. Kowalczyk and R. J. Le Roy, A full analytic potential energy curve for the $a^3\Sigma^+$ state of KLi from a limited vibrational data set, J. Chem. Phys. **126**, 194313 (2007).

[3] E. Tiemann, H. Knöckel, P. Kowalczyk, W. Jastrzebski, A. Pashov, H. Salami and A. J. Ross, Coupled system $a^3\Sigma^+$ and $X^1\Sigma^+$ of KLi: Feshbach resonances and corrections to the Born-Oppenheimer approximation, Phys. Rev. A **79**, 042716 (2009).

[4] M. Ivanova, A. Stein, A. Pashov, H. Knöckel and E. Tiemann, The $X^1\Sigma^+$ state of LiRb studied by Fourier-transform spectroscopy, J. Chem. Phys. **134**, 024321 (2011).

[5] G. Skrzyński and M. Musial, Benchmark study of the electronic states of the LiRb molecule: *Ab initio* calculations with the fock space coupled cluster approach, Molecules. **28**, 7645 (2023).

[6] P. Staanum, A. Pashov, H. Knöckel and E. Tiemann, $X^1\Sigma^+$ and $a^3\Sigma^+$ states of LiCs studied by Fourier-transform spectroscopy, Phys. Rev. A **75**, 042513 (2007).