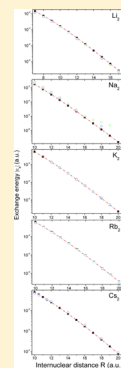


Calculating and Modeling the Exchange Energies of Homonuclear and Heteronuclear Alkali Dimers Based on the Surface Integral Method

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ABSTRACT: The exchange energies of all homonuclear and heteronuclear alkali dimers are calculated based on the surface integral method. These results are generally in good agreement with both ab initio calculations and experimental results where available. It is also shown that the exchange energies could be fitted by an analytical expression of $AR^b \exp(-cR)$. b and c can be calculated by two simple formulas that are only related to the ionization energies of the constituent atoms. A is the only parameter in this expression. More interestingly, it is found that the parameter A for the heteronuclear dimers could be approximated by a combining rule.



1. INTRODUCTION

Alkali metal molecular systems are of particular interest because they push the new development of cold and ultracold atomic trapping techniques, such as manipulation and control of ultracold chemical reactions,^{1–3} ultracold molecule collision dynamics,^{4–7} quantum computing,^{8,9} and experimental preparation of few-body quantum effects.¹⁰ A comprehensive way to calculate the exchange energy of alkali dimers is stimulated by these possible applications. Ab initio calculation and experiment are two prototype ways to obtain the exchange energy. However, these energy levels are calculated separately, and the exchange energy is obtained from the difference of two large numbers, resulting in a large relative error. The computational effort is usually very large, and the results can be found in only numerical form. At large R , the exchange energy $\epsilon_x = 1/2(\epsilon_s - \epsilon_t)$, loses significance because of a small difference between two large numbers. Here, ϵ_s and ϵ_t are the energy of the singlet state and triplet state, respectively. Thus, there has been considerable interest in developing the surface integral method, which leads to the exchange energy directly.

A detailed description of the development of the surface integral method for diatomic systems has been published elsewhere.^{11–13} In the case of two atoms, the surface integral method has since been successfully applied to calculating the exchange energies in H_2^+ ,¹⁴ H_2 ,¹² He_2 ,¹⁵ Ne_2 ,¹⁶ Ar_2 ,¹⁶ alkali hydrides,¹⁷ alkali helium systems,¹⁸ alkaline-earth-helium systems,¹⁹ and alkali dimer cations.²⁰ Although the exchange energies for alkali dimers based on the surface integral method have not yet been reported, the exchange energies of the homonuclear alkali dimers can be reduced to a simple formula $\epsilon_x = A(M, \beta)R^{(7/2\beta)-1} \exp(-2\beta R)$ according to Smirnov and Chibisov.²¹ One can find that the most difficult

part in the surface integral method is how to determine the parameter $A(M, \beta)$.

In this paper, we calculate the exchange energies of all alkali homonuclear and heteronuclear dimers based on the surface integral method. For the heteronuclear dimers, the β is obtained by the average value of the constituted atoms. It is shown that the analytical formula $AR^{(7/2\beta)-1} \exp(-2\beta R)$ can fit not only the exchange energies of homonuclear dimers but also those of heteronuclear dimers. Interestingly, the parameter A in the heteronuclear dimers can be approximated by a simple combining rule related to the corresponding homonuclear dimers. In the next section, a simple introduction to the surface integral method is presented. In section 3, the exchange energies of all alkali homonuclear and heteronuclear dimers are calculated. A simple analytical formula used to reproduce all of the calculation results is given in section 4. The paper is closed with a conclusion in the last section. Atomic units are used throughout.

2. SURFACE INTEGRAL METHOD

In the surface integral method, the exchange energy of a simple atom–atom system is directly related to the flux of valence electrons flowing back and forth between nuclei X and Y¹¹

$$\epsilon_x = \frac{-\int_{\Sigma} (\nabla \phi_a) \cdot \vec{n} \, d^3s}{1 - 2 \int_{\text{far}} \phi_a^2 \, d^3r} \quad (1)$$

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where ϕ_a is the localized wave function around nucleus X. The localized wave function can be written as the product of two atomic outermost valence $\psi_0(r)$.²² At large distances, the wave function of the atomic valence electron is the solution of the equation

$$\left[-\frac{1}{2}\nabla^2 + V_0(r) + E_1\right]\psi_0 = 0 \quad (2)$$

where E_1 is the ionization energy and $V_0(r)$ is the effective potential due to all other electrons and the nucleus. An analytical form of $\psi_0(r)$ can be derived in the long-range asymptotic region, where $V_0(r) \rightarrow -1/r$. The solution can be expressed in terms of the Whittaker function. The radial part is given by²³

$$\psi_0(r) = Mr^{(1/\beta)-1}e^{-\beta r}\left(1 + \sum_{t=1}^{\infty} \frac{a_t}{r^t}\right) \quad (3)$$

with

$$a_1 = \frac{1}{2\beta}\left[l(l+1) - \frac{1}{\beta}\left(\frac{1}{\beta} - 1\right)\right] \quad (4)$$

and

$$a_t = a_{t-1}\frac{1}{2\beta t}\left[l(l+1) - \left(\frac{1}{\beta} - t\right)\left(\frac{1}{\beta} - t + 1\right)\right] \quad (5)$$

where M is the amplitude and l is the orbital angular momentum of the valence electron, and

$$\beta = \sqrt{2E_1} \quad (6)$$

For a valence electron with $l = 0$, the wave function is simply

$$\phi = \frac{1}{\sqrt{4\pi}}\psi_0(r) \quad (7)$$

With this form of the asymptotic wave function, the surface integral of eq 1 leads to a simple expression for the exchange energy of a homonuclear diatomic molecule

$$\varepsilon_x = A(M, \beta)R^{(7/2\beta)-1}\exp(-2\beta R) \quad (8)$$

where

$$A(M, \beta) = \frac{1}{2}M^4\Gamma\left(\frac{1}{2\beta}\right)2^{-1-(1/\beta)}\beta^{-2-(1/2\beta)} \times \int_0^1 \exp\left(\frac{y-1}{\beta}\right)(1-y)^{3/2\beta}(1+y)^{1/2\beta} dy \quad (9)$$

The ionization energy entering into this expression can be obtained from eq 6, and the only other parameter is M , the amplitude of the asymptotic atomic wave function defined in eq 3. Thus, the otherwise complicated determination of the exchange energy between two equivalent atoms is drastically reduced to simply calculating the asymptotic amplitude M of the wave function of a single electron of an isolated atom.

For a heteronuclear dimer, the ionization energies and the amplitudes of the wave function for the two atoms will be different. β and M are defined for the first atom and α and N for the second atom. If α and β are not too different, the expression for its exchange energy is

$$\varepsilon_x = R^{(2/\alpha)+(2/\beta)-[1/(\alpha+\beta)]-1}\exp[-(\alpha+\beta)R]F(\alpha, \beta, R) \quad (10)$$

where

$$F(\alpha, \beta, R) = \frac{1}{2}M^2N^22^{-2-[2/(\alpha+\beta)]}\Gamma\left(\frac{1}{\alpha+\beta}\right) \times \left(\frac{2}{\alpha+\beta}\right)^{2+[1/(\alpha+\beta)]} [H(\alpha, \beta, R) + H(\beta, \alpha, R)] \quad (11)$$

$$H(\alpha, \beta, R) = \left(\frac{\alpha+\beta}{2\beta}\right)^{(2/\alpha)-2(\alpha+\beta)} \times \int_0^1 \exp\left(\frac{y-1}{\beta} + R(\beta-\alpha)y\right)(1-y)^{(2/\beta)-[1/(\alpha+\beta)]} \times (1+y)^{(2/\alpha)-(2/\beta)+[1/(\alpha+\beta)]} \left(1 + \frac{\beta-\alpha}{\beta+\alpha}y\right)^{-2-[1/(\alpha+\beta)]} dy \quad (12)$$

3. CALCULATING THE EXCHANGE ENERGIES OF ALL OF THE ALKALI HOMONUCLEAR AND HETERONUCLEAR DIMERS

According to eqs 8 and 12, the exchange energies for all alkali dimers are calculated. All of the parameters are listed in Table 1.

Table 1. Parameters of the Exchange Function (in atomic units) Taken Directly from Reference 21

system	β	M
Li	0.630	0.765
Na	0.626	0.751
K	0.567	0.553
Rb	0.556	0.491
Cs	0.536	0.416

The parameter β , which has been determined very accurately, is taken from the ref 21. The amplitude M for the alkali atoms is also taken directly from the ref 21, which was determined by the behavior of the wave functions of the electrons inside of the atoms. Smirnov et al. have shown that it can give very good results for the alkali dimers. The absolute value of the exchange energies $|\varepsilon_x|$ for all alkali dimers based on the present method are displayed in Figures 1 and 2. Moreover, we also show the relevant ab initio calculations and experimental results where available.

For Li_2 , Zemke and Stwalley²⁴ determined the exchange energy contributions to the intermediate and long-range interaction potentials based on the experimental results of the two lowest states of Li_2 . It is gratifying to see that the present results are in good agreement with Zemke's experimental results. There is also an ab initio calculation for this system.²⁵ As an illustration, the ab initio results and the experimental results agree almost exactly. It is not a surprise that our results are in accord with these ab initio results. For Na_2 , by comparing our results with the MC-SCF (multiconfiguration self-consistent field) calculations²⁶ and experimental results,²⁷ one can see that the excellent agreement is seen to be under $R = 17$ au. However, there are noticeable discrepancies for $R > 18$ au. It is not true that the long-range portion of the potential is less accurate than the shorter range; this is principally due to recent ultracold molecule experiments. Therefore, noticeable discrepancies at this range are considered to be reasonable. Using the perturbation-facilitated optical-optical double resonance (PFOODR) technique, Zhao et al. obtained an improved triplet K_2 potential, which eliminated the crossing problem. By combining these triplet results and the

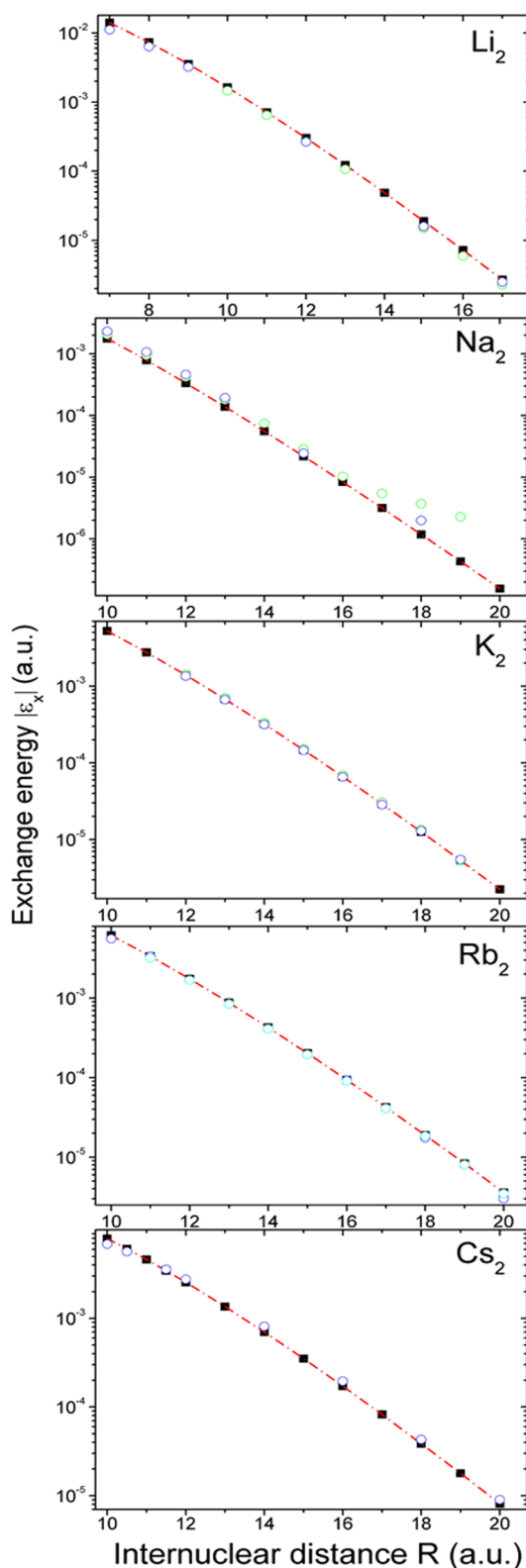


Figure 1. The exchange energies of homonuclear alkali dimers. The black solid square, green hollow circle, blue hollow circle, and red dashed-dotted line represent the present, experimental, ab initio calculation, and fitted results, respectively. The cyan hollow circle represents the results determined by the analytical expression according to ref 21.

previous ground-state results, an improved analysis of long-range exchange interactions between two K atoms was reported.²⁸ The

K_2 results based on the surface integral method agree well with the reported experimental results²⁸ and ab initio calculation results.²⁹ For Rb_2 , Strauss et al.³⁰ have reported the exchange contribution for $R > 11$ au by quite accurate experimental results. Figure 1 shows that the present Rb_2 results agree well with the results reported by Strauss et al.³⁰ In addition, excellent agreement between the present Rb_2 and Cs_2 results and CEP+CPP (compact effective potentials and core polarization potentials) calculations³¹ is exhibited. From the above-mentioned, we can predict that the surface integral method is able to provide remarkably accurate exchange energies for homonuclear alkali dimers.

As shown in section 2, the surface integral method used in this paper for the heteronuclear and homonuclear dimers should have the same accuracy. Because this method is very accurate for the homonuclear alkali dimers, our heteronuclear dimer results should also be pretty good. This is indeed the case. As shown in Figure 2, the LiCs results are in good agreement with the full configuration interaction calculation results.³² For NaK, the present results are in excellent agreement with not only the ab initio results²⁹ but also experimental results.³³ For KRb, our results are presented to compare with the exchange contribution for $R > 11$ au reported by Pashov et al.³⁴ The present results agree well with their results. Zemke and Stwalley³⁵ reported the exchange energy of NaRb for $R > 13.5788$ au determined from the ab initio full valence configuration interaction calculations of the $X^1\Sigma^+$ and $a^3\Sigma^+$ state potentials by Korek et al.³⁶ Our results and their results agree very well with each other. Moreover, the present results for NaRb and NaCs are also in very good agreement with the ab initio results of Aymar and Dulieu.³⁷ Therefore, the exchange energies obtained in this paper based on the surface integral method should be believable.

4. MODELING THE EXCHANGE ENERGIES OF ALL OF THE ALKALI HOMONUCLEAR AND HETERONUCLEAR DIMERS

It is possible to model the exchange energies of all of the alkali homonuclear and heteronuclear dimers. Zemke and Stwalley³⁸ found a simple and reliable formula for the determination of exchange energies from intermediate to large R values for Li_2 , Na_2 , K_2 , and NaK . In section 2, eq 8 shows that the exchange energies of the homonuclear dimers could also be reduced to a simple analytical formula

$$\epsilon_x = AR^b e^{-cR} \quad (13)$$

Here, $b = (7/2\beta) - 1$, and $c = 2\beta$. This analytical expression and the expression mentioned in ref 38 are both according to Smirnov and Chibisov.²¹ Here, we assume that the exchange energies of all of the alkali homonuclear and heteronuclear dimers could be fitted by eq 13. For the heteronuclear dimers, the β is obtained from the average value of the constituent atoms. Therefore, there is only one parameter A that has to be determined. Figures 1 and 2 show the results. One can clearly see that all of the exchange energies can be closely fitted with eq 13. Table 2 lists the fitting values of A . A_{surf} , A_{exp} , and $A_{ab initio}$ mean that the fitted values are determined from the surface integral methods, experimental, and ab initio results, respectively. The A_{exp} values for Li_2 , Na_2 , K_2 , and NaK are in fairly good agreement with those in the ref 38. Maybe there is another way to determine parameter A for the heteronuclear alkali dimers. From eq 9, it is shown that A is closely related to the parameter β . Therefore, we

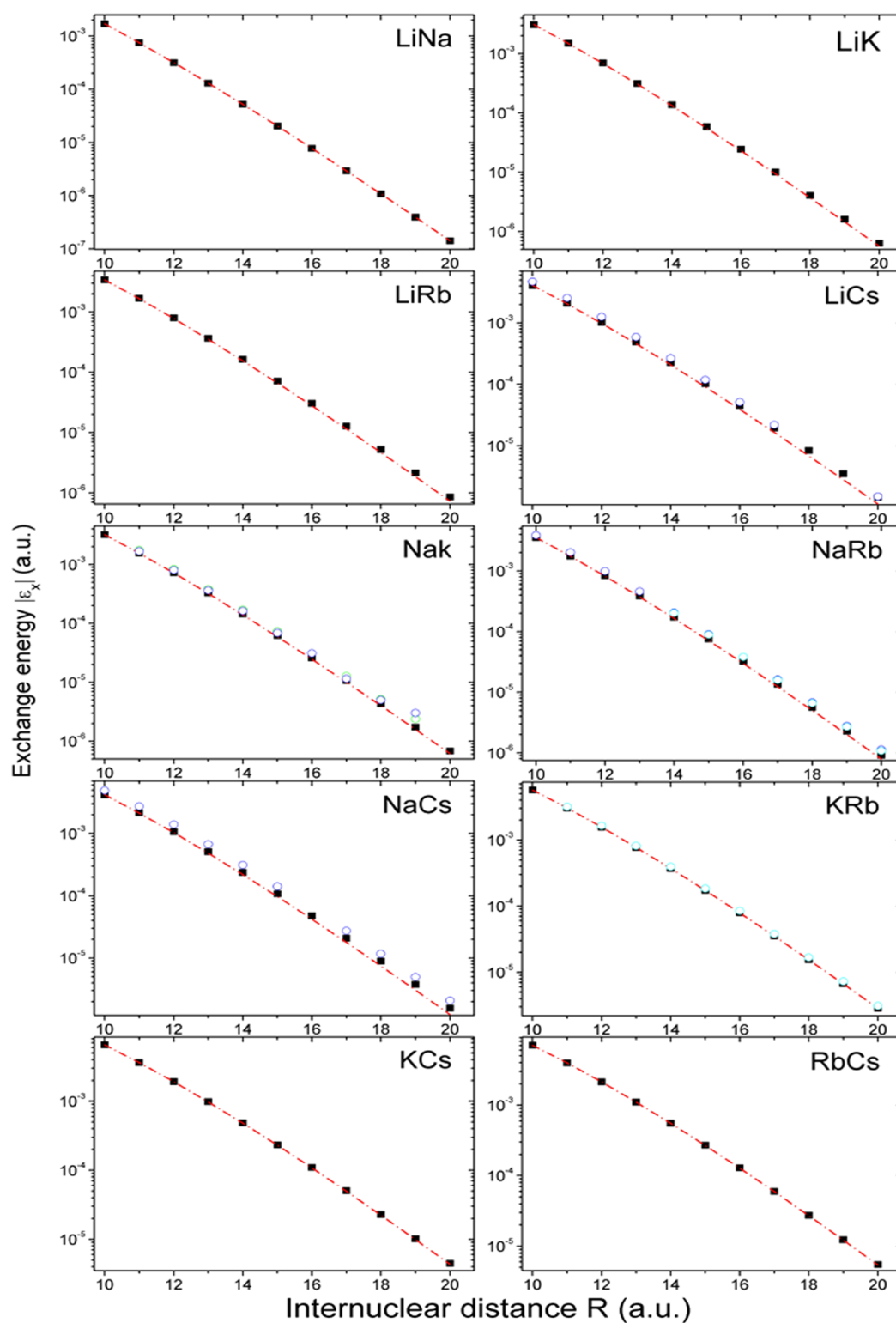


Figure 2. The exchange energies of heteronuclear alkali dimers. The black solid square, green hollow circle, blue hollow circle, and red dashed–dotted line represent the present, experimental, ab initio calculation, and fitted results, respectively. The cyan hollow circle represents the results determined by the analytical expression according to ref 21.

suppose that A for the heteronuclear dimers can be determined by the corresponding homonuclear dimers based on the following simple formula.

$$A_{XY} = \frac{\alpha N}{\beta M + \alpha N} A_{XX} + \frac{\beta M}{\beta M + \alpha N} A_{YY} \quad (14)$$

Here, A_{XX} and A_{YY} represent the homonuclear dimers XX and YY , respectively. The A_{XY} represents the value A for the heteronuclear dimer after the combining by eq 14. In Table 2, we also list the calculation results using eq 14. It is clearly shown that eq 14 is a very good approximation to the A of the heteronuclear dimers. The largest relative error is only 6.33%.

Table 2. A_{surf} Representing the Exchange Energies Calculated by the Surface Integral Method along with A_{exp} and $A_{\text{ab initio}}$ as the Exchange Energies Calculated by the Experimental and Ab Initio Results, Respectively^a

dimer	A_{surf}	A_{exp}	$A_{\text{ab initio}}$	A_{XY}
Li ₂	0.01346	0.01099	0.01092	
Na ₂	0.01245	0.00925	0.01034	
K ₂	0.00296	0.00273	0.00259	
Rb ₂	0.00211		0.00178	
Cs ₂	0.00106		0.00093	
LiNa	0.01295			0.01295
LiK	0.00694			0.00701
LiRb	0.00607			0.00621
LiCs	0.00470		0.00588	0.00498
NaK	0.00660	0.00571	0.00547	0.00668
NaRb	0.00577		0.00497	0.00591
NaCs	0.00444		0.00433	0.00473
KRb	0.00251			0.00251
KCs	0.00182			0.00187
RbCs	0.00151			0.00153

^a A_{XY} is the result of eq 14.

5. CONCLUSION

In this paper, we have calculated the exchange energies of the heteronuclear and homonuclear alkali dimers based on the surface integral method. Our results agree well with the ab initio and experimental results. We also find that all of the exchange energies can be closely fitted with a single-parameter analytical formula. It is interesting to see that the only parameter in the heteronuclear dimer systems could be determined by the corresponding homonuclear dimer systems. We hope that this observation will be useful for the development of the combining rule in the potential model field.

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Notes

The authors declare no competing financial interest.

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REFERENCES

- (1) Balakrishnan, N.; Dalgarno, A. Chemistry at Ultracold Temperatures. *Chem. Phys. Lett.* **2001**, *341*, 652–656.
- (2) Bodo, E.; Gianturco, F. A.; Dalgarno, A. F+D₂ Reaction at Ultracold Temperatures. *J. Chem. Phys.* **2002**, *116*, 9222–9226.
- (3) Rom, T.; Best, T.; Mandel, O. State Selective Production of Molecules in Optical Lattices. *Phys. Rev. Lett.* **2004**, *93*, 073002–073005.
- (4) Kajita, M. Cold Collisions between Linear Polar Molecules. *Eur. Phys. J. D* **2003**, *23*, 337–342.
- (5) Krems, R. V. Molecules near Absolute Zero and External Field Control of Atomic and Molecular Dynamics. *Int. Rev. Phys. Chem.* **2005**, *24*, 99–118.
- (6) Avdeenkov, A. V.; Kajita, M.; Bohn, J. L. Suppression of Inelastic Collisions of Polar ¹Σ State Molecules in an Electrostatic Field. *Phys. Rev.* **2006**, *73*, 022707–022713.
- (7) Krems, R. V. Controlling Collisions of Ultracold Atoms with dc Electric Fields. *Phys. Rev. Lett.* **2006**, *96*, 123202/1–123202/4.

(8) Demille, D. Quantum Computation with Trapped Polar Molecules. *Phys. Rev. Lett.* **2002**, *88*, 067901/1–067901/4.

(9) Yelin, S. F.; Kirby, K.; Côté, R. Dipolar Switching for Robust Quantum Computation with Polar Molecules. *arXiv:quant-ph/0602030* **2006**, 0602030

(10) Kraemer, T.; Mark, M.; Walburger, P.; Danzl, J. G.; Chin, C.; Engesser, B.; Lange, A. D.; Pilch, K.; Jaakkola, A.; Nagerl, H. C.; Grimm, R. Evidence for Efimov Quantum States in an Ultracold Gas of Caesium Atoms. *Nature* **2006**, *440*, 315–318.

(11) Tang, K. T.; Toennies, J. P.; Yiu, C. L. The Generalized Heitler–London Theory for Interatomic Interaction and Surface Integral Method for Exchange Energy. *Int. Rev. Phys. Chem.* **1998**, *17*, 363–406.

(12) Tang, K. T.; Toennies, J. P.; Yiu, C. L. Exchange Energy of H₂ Calculated by the Surface Integral Method in Zeroth Order Approximation. *J. Chem. Phys.* **1993**, *99*, 377–388.

(13) Bouty, O.; Hädinger, G.; Aubert-Frécon, M. Exchange Interaction Energy between Two One-Active Electron Atoms at Large Distances. *J. Mol. Struct.* **1995**, *330*, 97–106.

(14) Tang, K. T.; Toennies, J. P.; Yiu, C. L. The Exchange Energy of H₂⁺ Calculated from Polarization Perturbation Theory. *J. Chem. Phys.* **1991**, *94*, 7266–7277.

(15) Tang, K. T.; Toennies, J. P.; Yiu, C. L. Accurate Analytical He–He van der Waals Potential Based on Perturbation Theory. *Phys. Rev. Lett.* **1995**, *74*, 1546–1549.

(16) Kleinekathöfer, U.; Tang, K. T.; Toennies, J. P.; Yiu, C. L. Van der Waals Potentials of He₂, Ne₂, and Ar₂ with the Exchange Energy Calculated by the Surface Integral Method. *J. Chem. Phys.* **1997**, *107*, 9502–9513.

(17) Yiu, C. L.; Tang, K. T.; Greenwood, W. G. Asymptotic Exchange Energy of Heteronuclear Dimers. *J. Phys. Chem. A* **2011**, *115*, 7346–7351.

(18) Kleinekathöfer, U.; Tang, K. T.; Toennies, J. P.; Yiu, C. L. Potentials for Some Rare Gas and Alkali–Helium Systems Calculated from the Surface Integral Method. *Chem. Phys. Lett.* **1996**, *249*, 257–263.

(19) Kleinekathöfer, U. Ground State Potentials for Alkaline-Earth Helium Diatoms Calculated by the Surface Integral Method. *Chem. Phys. Lett.* **2000**, *324*, 403–410.

(20) Johann, C.; Kleinekathöfer, U.; Tang, K. T.; Toennies, J. P. Generalized Heitler–London Theory with Exchange Energy by the Surface Integral Method: an Application to the Alkali Metal Dimer Cations. *Chem. Phys. Lett.* **1996**, *257*, 651–657.

(21) Smirnov, B. M.; Chibisov, M. I. Electron Exchange and Changes in the Hyperfine State of Colliding Alkaline Metal Atoms. *Sov. Phys. JETP* **1965**, *21*, 624–628.

(22) Hädinger, G.; Hädinger, G.; Magnier, S.; Frecon, M. A. A Particular Case of Asymptotic Formulas for Exchange Energy between Two Long-Range Interacting Atoms with Open Valence Shells of Any Type: Application to the Ground State of Alkali Dimers. *J. Mol. Spectrosc.* **1996**, *175*, 441–444.

(23) Bates, D. R.; Damgaard, A. The Calculation of the Absolute Strengths of Spectral Lines. *Phil. Trans. R. Soc. London, Ser. A* **1949**, *242*, 101–122.

(24) Zemke, W. T.; Stwalley, W. C. Analysis of Long-Range Dispersion and Exchange Interactions of Two Lithium Atoms. *J. Phys. Chem.* **1993**, *97*, 2053–2058.

(25) Schmidt-Mink, I.; Müller, W.; Meyer, W. Ground- and Excited-State Properties of Li₂ and Li₂⁺ from *Ab Initio* Calculations with Effective Core Polarization Potentials. *Chem. Phys.* **1985**, *92*, 263–285.

(26) Konowalow, D. D.; Rosenkrantz, M. E. Long-Range Interactions of Sodium (3s²S) with Sodium (3s²S) or Sodium (3p²P). *J. Phys. Chem.* **1982**, *86*, 1099–1102.

(27) Zemke, W. T.; Stwalley, W. C. Analysis of Long Range Dispersion and Exchange Interactions between Two Na Atoms. *J. Chem. Phys.* **1994**, *100*, 2661–2670.

(28) Zhao, G.; Zemke, W. T.; Kim, J. T.; Ji, B.; Wang, H.; Bahns, J. T.; Stwalley, W. C.; Li, L.; Lyrra, A. M.; Amiot, C. New Measurements of the a³Σ_u⁺ State of K₂ and Improved Analysis of Long Range Dispersion and

Exchange Interactions between Two K Atoms. *J. Chem. Phys.* **1996**, *105*, 7976–7985.

(29) (a) Magnier, S. Ph. D. Thesis, University of Paris, Orsay, France, 1993. (b) Magnier, S.; Millie, Ph. Potential Curves for the Ground and Numerous Highly Excited Electronic States of K_2 and NaK. *Phys. Rev. A* **1996**, *54*, 204–218.

(30) Strauss, C.; Takekoshi, T. Hyperfine, Rotational, and Vibrational Structure of the $a^3\Sigma_u^+$ State of $^{87}\text{Rb}_2$. *Phys. Rev. A* **2010**, *82*, 052514/1–052514/12.

(31) Krauss, M.; Stevens, W. J. Effective Core Potentials and Accurate Energy Curves for Cs_2 and Other Alkali Diatomics. *J. Chem. Phys.* **1990**, *93*, 4236–4242.

(32) Mabrouk, N.; Berriche, H.; Ben Ouada, H. Theoretical Study of the LiCs Molecule: Adiabatic and Diabatic Potential Energy and Dipole Moment. *J. Phys. Chem. A* **2010**, *114*, 6657–6658.

(33) Zemke, W. T.; Stwalley, W. C. Analysis of Long Range Dispersion and Exchange Interactions between One Na atom and One K atom. *J. Chem. Phys.* **1999**, *111*, 4956–4961.

(34) Pashov, A.; Docenko, O.; Tamanis, M. Coupling of the $X^1\Sigma^+$ and $a^3\Sigma^+$ States of KRb. *Phys. Rev. A* **2007**, *76*, 022511/1–022511/10.

(35) Zemke, W. T.; William, C. Stwalley Long-Range Potential Energy Curves for the $X^1\Sigma^+$ and $a^3\Sigma^+$ States of NaRb. *J. Chem. Phys.* **2001**, *114*, 10811–10815.

(36) Korek, M.; Allouche, A. R.; Kobeissi, M. Theoretical Study of the Electronic Structure of the LiRb and NaRb Molecules. *Chem. Phys.* **2000**, *256*, 1–6; the point wise potentials were from their website.

(37) Aymar, M.; Dulieu, O. Calculations of Transition and Permanent Dipole Moments of Heteronuclear Alkali Dimers NaK, NaRb and NaCs. *Mol. Phys.* **2007**, *105*, 1733–1742.

(38) Zemke, W. T.; Stwalley, W. C. Analysis of Exchange Energy at Long Range for States of Alkali Diatomic Molecules Correlating to Two Ground State Atoms. *J. Chem. Phys.* **1999**, *111*, 4962–4965.