Supporting Materials

Improved Pair-Potential Function for Diatomic Systems

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List of Contents

1. Alkaline-Earth Diatomic Systems

2. Rare-Gas Diatomic Systems:

3. Alkali-Helium Diatomic Systems

4. Group 12 Diatomic Systems

5. Reduced Potential Energy Curves: $U(R_s) = V(R)/De$ and $R_s = (R - R_e)/R_e$ Scheme

6. Reduced Potential Energy Curves: $U(R_s) = V(R)/De$ and $R^* = (R - R_e)/L_2$ Scheme

1 Alkaline-Earth Diatomic Systems

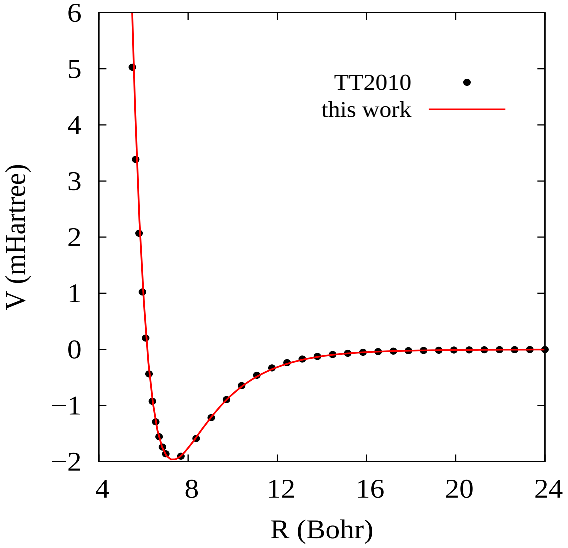

Fig.S1(a) The comparison between the new model potential (red line, this work, $\alpha = 1.05795181$, $\beta = 3.67097693$, $\gamma = 0.499242836$, $\eta = 17.4184595$, and $\zeta = 10.7$) and Tang-Toennies (TT2010)) potential (dark filled circles, Ref. [18]) for the ground-state $\mathbf{Mg}_2$. The potential energy $V(R) = E(R) - E_{\infty}$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 7.354 Bohr and -1.962 mHartree, respectively, of Ref. [18].

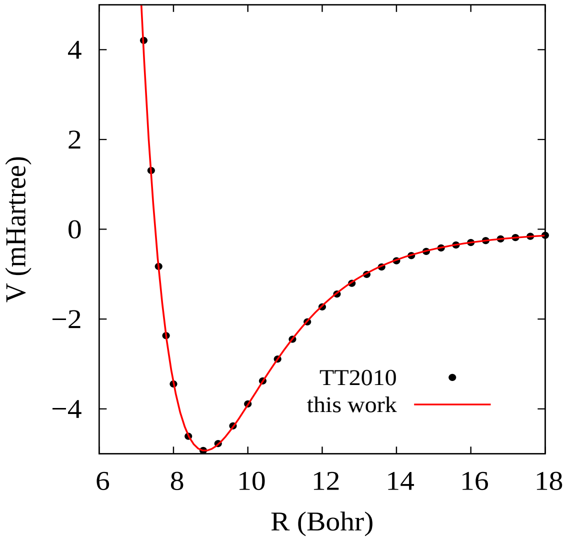

Fig.S1(b) The comparison between the new model potential (red line, this work, $\alpha = 0.785467116$, $\beta = 3.10926315$, $\gamma = 0.399101564$, $\eta = 26.5914016$, and $\zeta = 16.0$) and Tang-Toennies (TT2010)) potential (dark filled circles, Ref. [19]) for the ground-state $\mathbf{Sr}_2$. The potential energy $V(R) = E(R) - E_{\infty}$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 8.848 Bohr and -4.933mHartree, respectively, of Ref. [19].

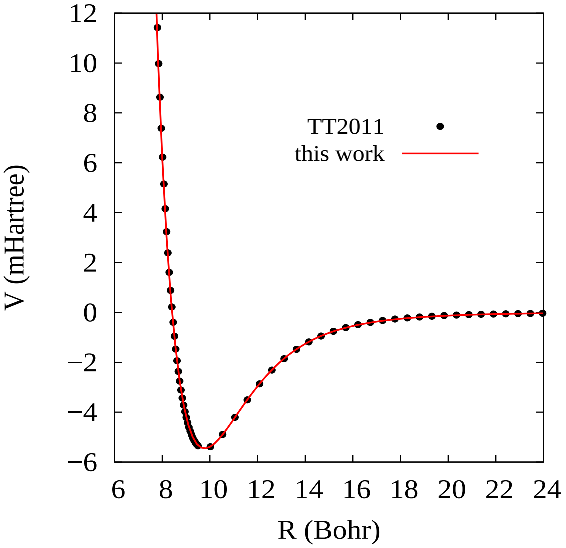

Fig.S1(c) The comparison between the new model potential (red line, this work, $\alpha = 0.685979692$, $\beta = 0.960619083$, $\gamma = 0.475823144$, $\eta = 83.3087266$, and $\zeta = 17.0$) and Tang-Toennies (TT2011)) potential (dark filled circles, Ref. [20]) for the ground-state $\mathbf{Ba}_2$. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 9.768 Bohr and -5.461mHartree, respectively, of Ref. [20].

2 Rare-Gas Diatomic Systems: Ar_2, Kr_2

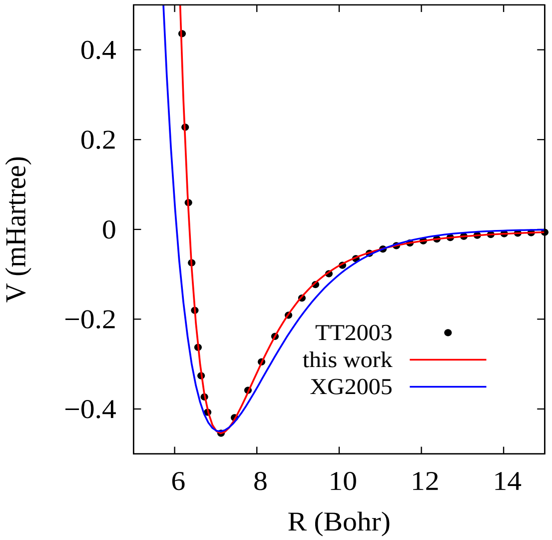

Fig.S2(a) The comparison between the new model potential (red line, this work, $\alpha = 1.41971509$, $\beta = 13.4773495$, $\gamma = 0.704291784$, $\eta = 80.9966379$, and $\zeta = 10.2$), three-parameter potential (XG2005) (blue line, $\alpha = 0.8706$, $\beta = 0.403498$, $\gamma = 0.38$, Ref. [23]) and Tang-Toennies (TT2003)) potential (dark filled circles, Ref. [15]) for the ground-state $\mathbf{Ar_2}$. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 7.10 Bohr and -0.454mHartree, respectively, of Ref. [15].

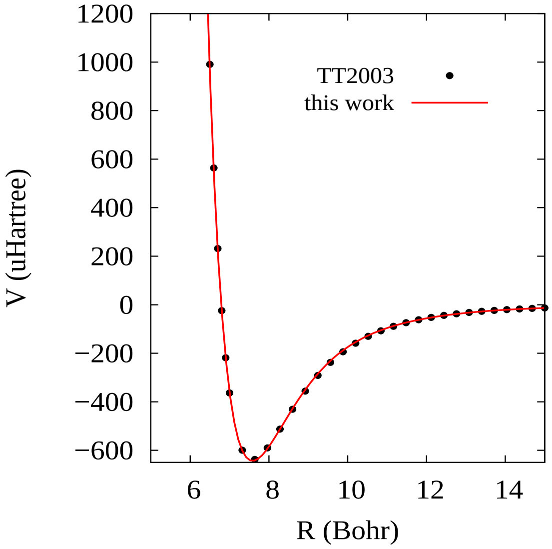

Fig.S2(b) The comparison between the new model potential (red line, this work, $\alpha = 1.35607455$, $\beta = 8.7269567$, $\gamma = 0.765828689$, $\eta = 206.380386$, and $\zeta = 10.3$) and Tang-Toennies (TT2003)) potential (dark filled circles, Ref. [15]) for the ground-state $\mathbf{Kr_2}$. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 7.58 Bohr and -638μHartree, respectively, of Ref. [15].

3 Alkali-Helium Diatomic Systems

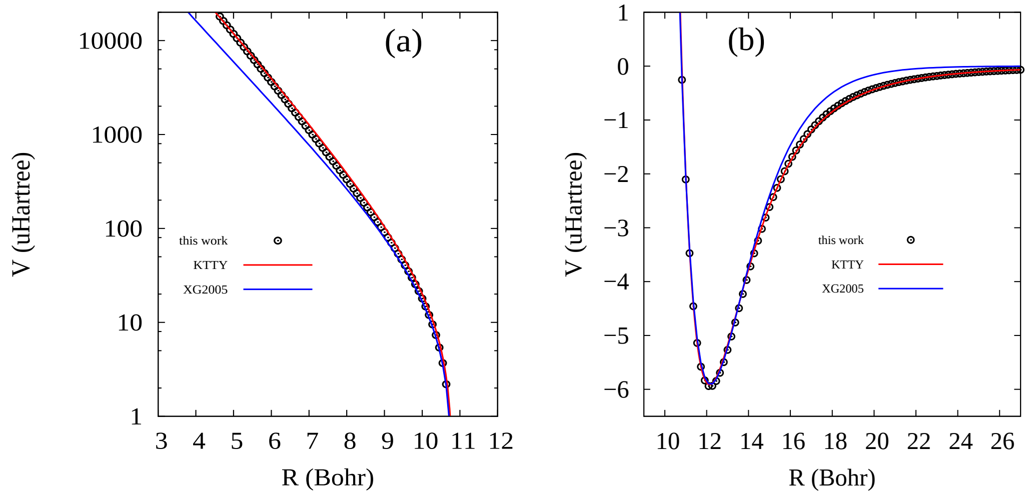

Fig.S3 The comparison between the new model potential (dark circles, this work, $\alpha = 0.6949$, $\beta = 0.00874$, $\gamma = 0.69$, $\eta = 8.1$, and $\zeta = 19.3$), three-parameter potential (XG2005) (blue line, $\alpha = 0.678$, $\beta = 0.00863$, $\gamma = 0.69$, Ref. [23]) and Kleinekathöfer-Tang-Toennies-Yiu (KTTY) potential (red line, Ref. [11]) for the weakly bound **NaHe**. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 12.155 Bohr and -5.91μHartree, respectively, of Ref. [11]. (a) Short-R region (Energy in log scale); (b) Intermediate- and Large-R regions.

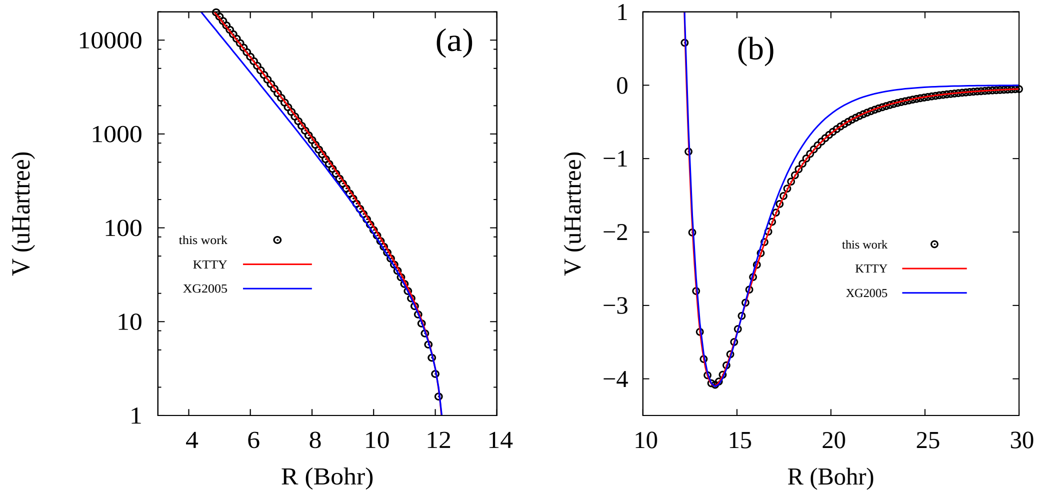

Fig.S4 The comparison between the new model potential (dark circles, this work, $\alpha = 0.645$, $\beta = 0.007177$, $\gamma = 0.55$, $\eta = 3.2$, and $\zeta = 19.95$), three-parameter potential (XG2005) (blue line, $\alpha = 0.615$, $\beta = 0.00679$, $\gamma = 0.55$, Ref. [23]) and Kleinekathöfer-Tang-Toennies-Yiu ((KTTY)) potential (red line, Ref. [11]) for the weakly bound **KHe**. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 13.8Bohr and -4.093μHartree, respectively, of Ref. [11]. (a) Short-R region (Energy in log scale); (b) Intermediate- and Large-R regions.

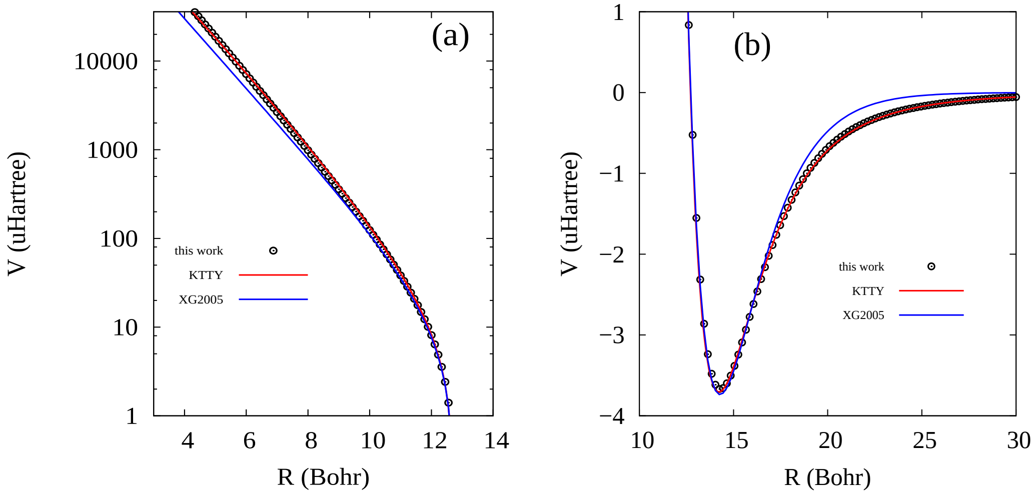

Fig.S5 The comparison between the new model potential (dark circles, this work, $\alpha = 0.6158$, $\beta = 0.00644$, $\gamma = 0.55$, $\eta = 3.01$, and $\zeta = 22.0$), three-parameter potential (XG2005) (blue line, $\alpha = 0.599$, $\beta = 0.00632$, $\gamma = 0.55$, Ref. [23]) and Kleinekathöfer-Tang-Toennies-Yiu ((KTTY)) potential (red line, Ref. [11]) for the weakly bound **RbHe**. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 14.234Bohr and -3.704μHartree, respectively, of Ref. [11]. (a) Short-R region (Energy in log scale); (b) Intermediate- and Large-R regions.

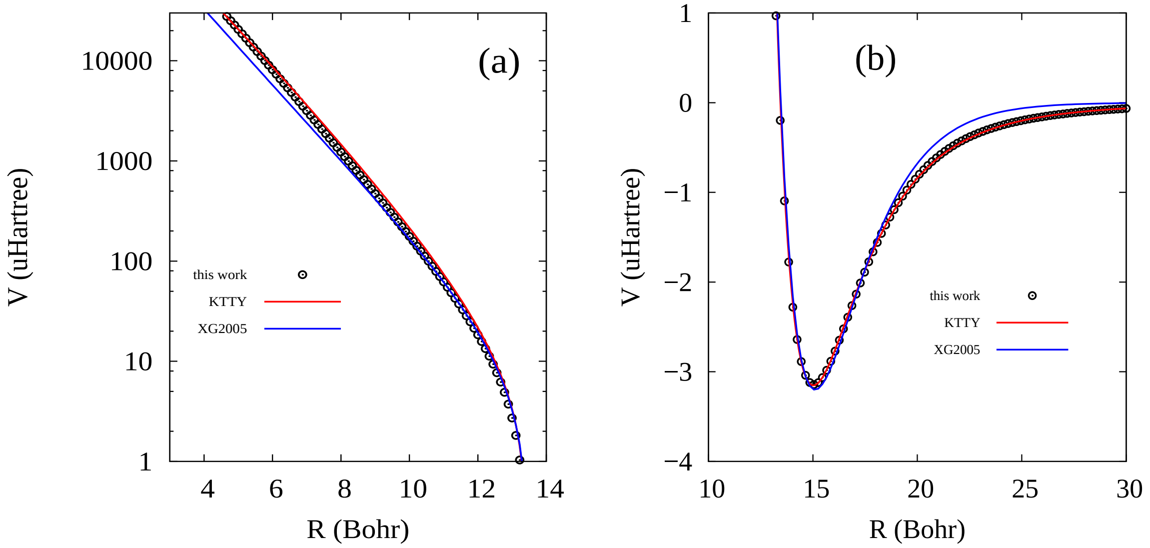

Fig.S6 The comparison between the new model potential (dark circles, this work, $\alpha = 0.5885$, $\beta = 0.005643$, $\gamma = 0.546$, $\eta = 3.25$, and $\zeta = 23.0$), three-parameter potential (XG2005) (blue line, $\alpha = 0.571$, $\beta = 0.00559$, $\gamma = 0.546$, Ref. [23]) and Kleinekathöfer-Tang-Toennies-Yiu ((KTTY)) potential (red line, Ref. [11]) for the weakly bound **CsHe**. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 15.028 Bohr and -3.151μHartree, respectively, of Ref. [11]. (a) Short-R region (Energy in log scale); (b) Intermediate- and Large-R regions.

4 Group 12 Diatomic Systems

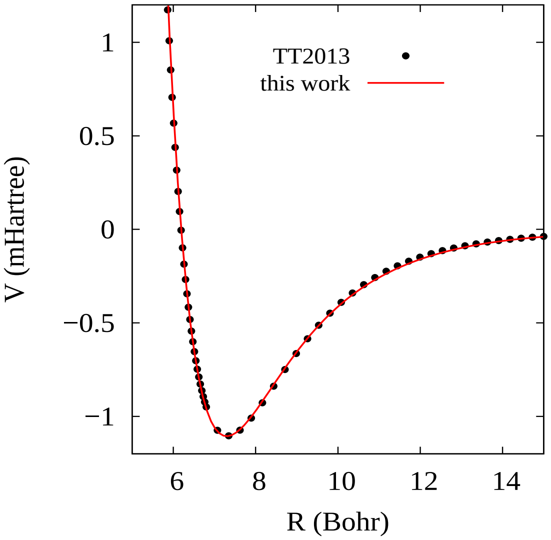

Fig.S7(a) The comparison between the new model potential (red line, this work, $\alpha = 1.04950583$, $\beta = 0.89490001$, $\gamma = 0.5675643$, $\eta = 10.5555675$, and $\zeta = 10.6$) and Tang-Toennies (TT2013)) potential (dark filled circles, Ref. [22]) for the ground-state $\mathbf{Zn}_2$. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 7.323 Bohr and -1.10mHartree, respectively, of Ref. [22].

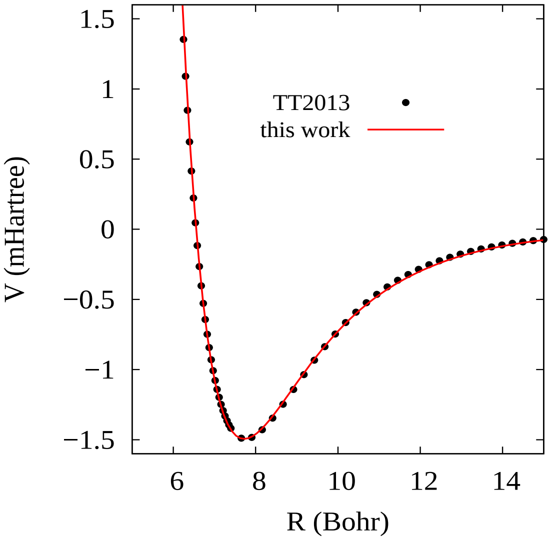

Fig.S7(b) The comparison between the new model potential (red line, this work, $\alpha = 1.02411942$, $\beta = 1.77266453$, $\gamma = 0.526618617$, $\eta = 15.7820342$, and $\zeta = 11.0$) and Tang-Toennies (TT2013)) potential (dark filled circles, Ref. [22]) for the ground-state $\mathbf{Cd}_2$. The potential energy $V(R) = E(R) - E_\infty$. The equilibrium distance R_e and minimum energy V_{min} in the new model potentials are fitted to 7.752 Bohr and -1.49mHartree, respectively, of Ref. [22].

5 Reduced Potential Curve: $R_s = (R - R_e)/R_e$ Scheme

Is it possible to find a simple globally accurate function for potential curves away from the vicinity of the equilibrium distance R_e for van der Waals diatomic systems? To answer this question, we test the global universality of the closed form expression Eq.(2) for the systems investigated above. The following figures presents the results based on the scaling scheme with a dimensionless length $Rs = (R - R_e)/R_e$ [27]. Figure 12(a), Fig.12(b), or Fig.12(c) show that both Rare-gas and Alkli-Rare-Gas systems, the Alkaline-Earth systems, or Group 12 systems seem to present a single binding energy relation, respectively. However, All these systems do not support a single binding-energy relation.

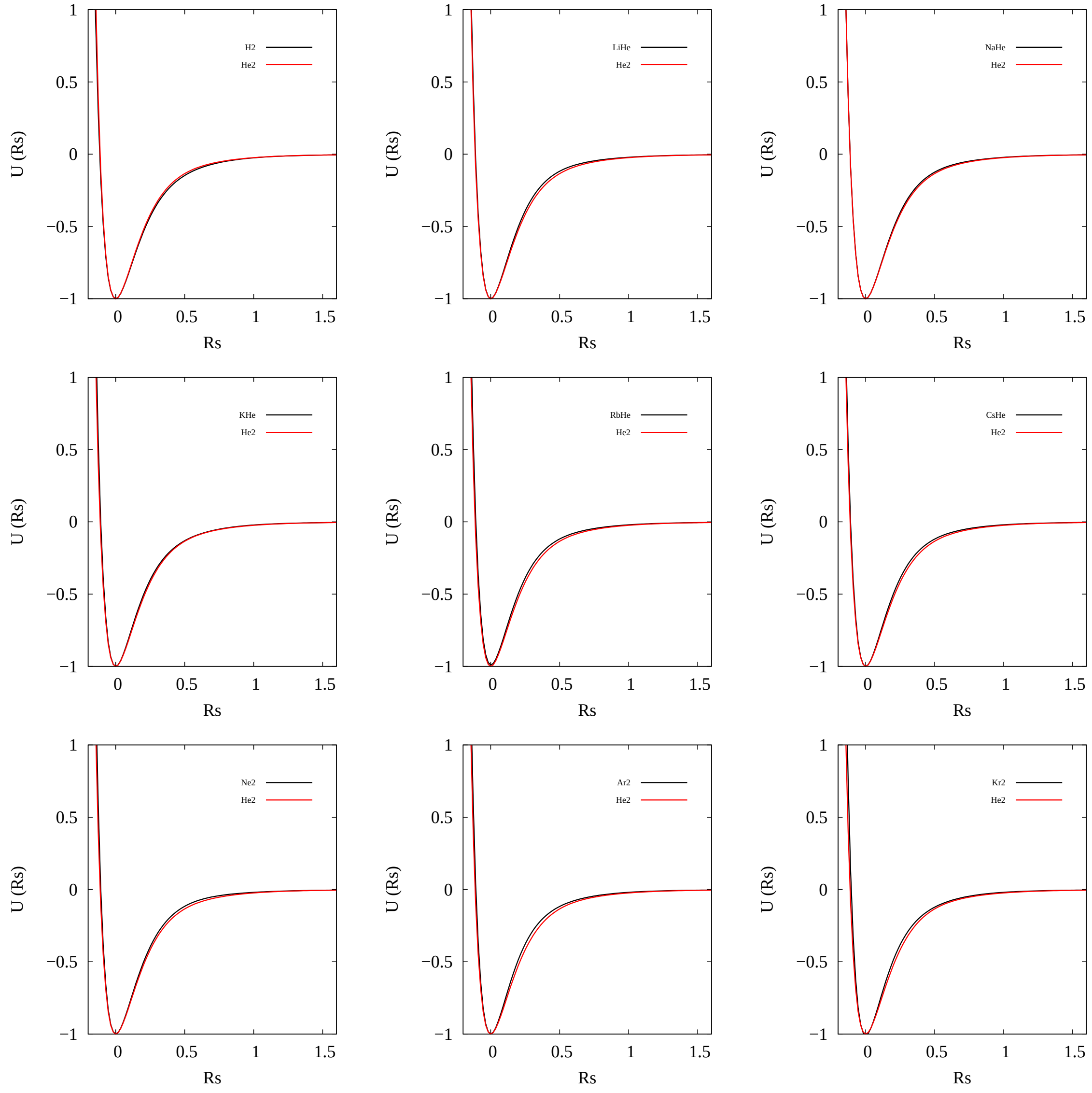

Fig.S8(a) Reduced potential curves $U(R_s) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$)for He_2, Ne_2,Ar_2, Kr_2, H_2 ($^3\sum$ state), LiHe, NaHe, KHe,RbHe, and CsHe with $R_s = (R - R_e)/R_e$. All are referenced to He_2. These systems seem to support a single binding energy relation.

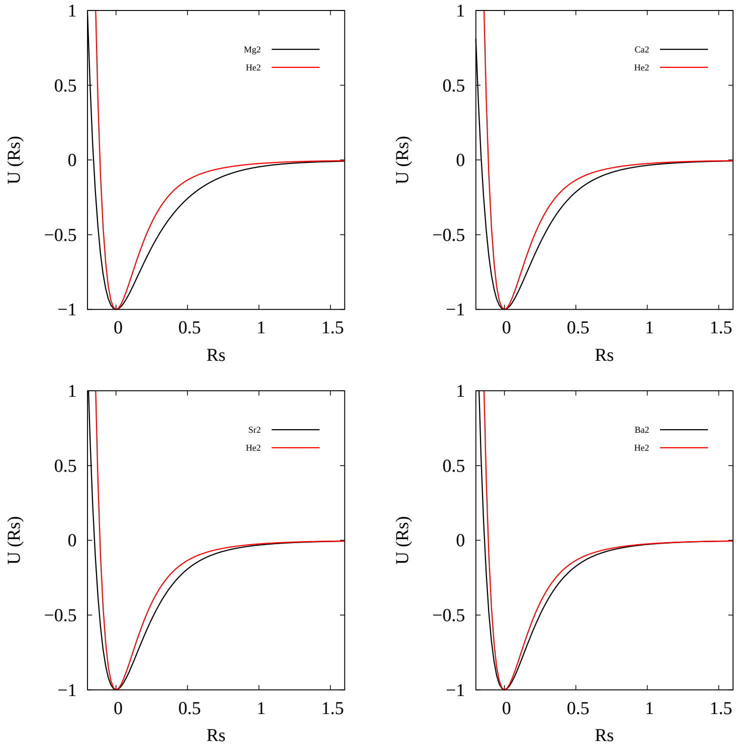

Fig.S8(b) Reduced potential curves $U(R_s) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$)for Alkaline-earth systems Mg_2, Ca_2, Sr_2, and Ba_2 with $R_s = (R - R_e)/R_e$. All are referenced to He_2. These Alkaline-earth systems seem to support a single binding energy relation.

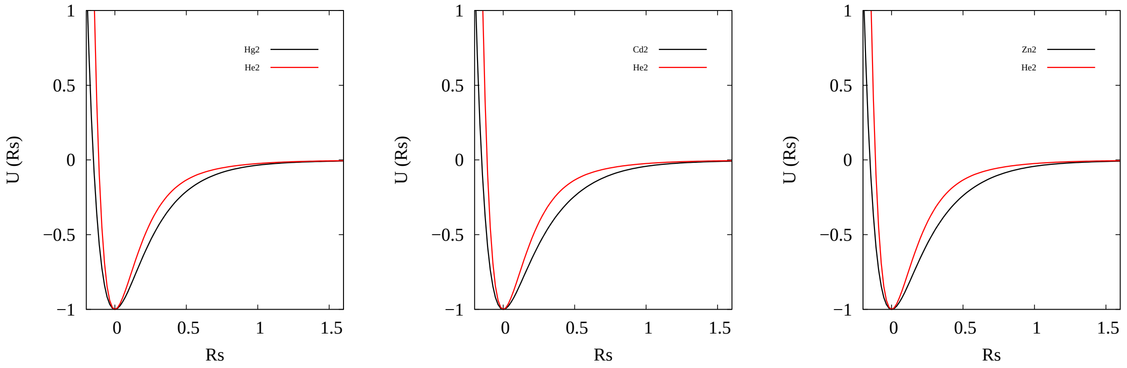

Fig.S8(c) Reduced potential curves $U(R_s) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$)for the group 12 systems: Cd_2, Zn_2, and Hg_2 with $R_s = (R - R_e)/R_e$. All are referenced to He_2. These group 12systems seem to support a single binding energy relation.

6 Reduced Potential Curve: $R^* = (R - R_e)/L_2$ Scheme

Using the dimensionless length $R^* = (R - R_e)/L_2$, we find that all the diatomic systems studied in this Note, as shown in Fig.13 to Fig.27, can have a universal reduced potential curve in the well region and long-range region away from the vicinity of the equilibrium distance R_e.

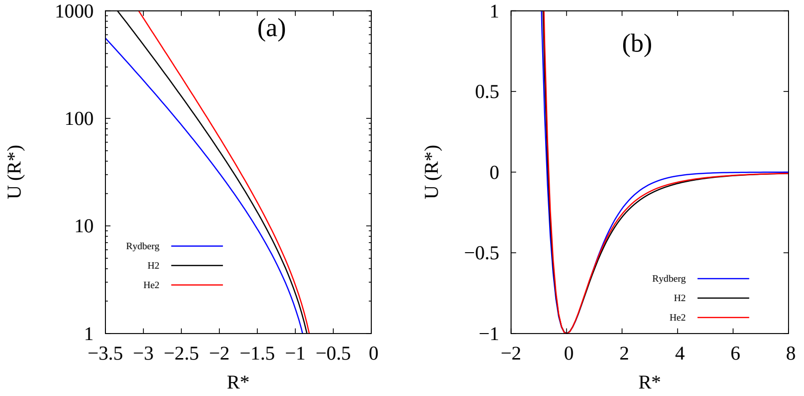

Fig.S9 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He_2, H_2 ($^3\sum$ state), and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

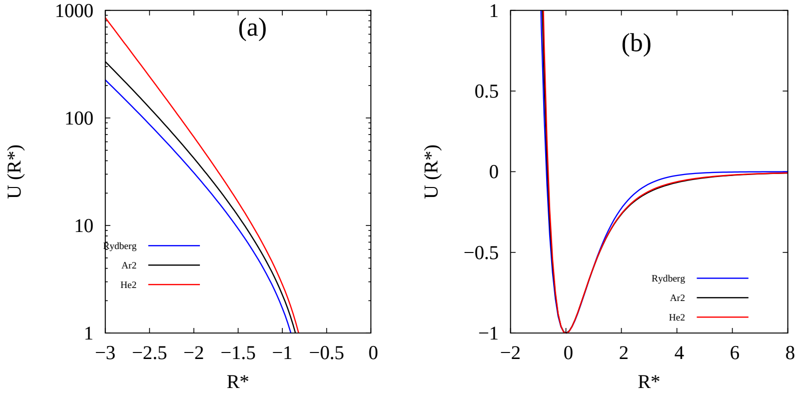

Fig.10 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He_2, Ar_2, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

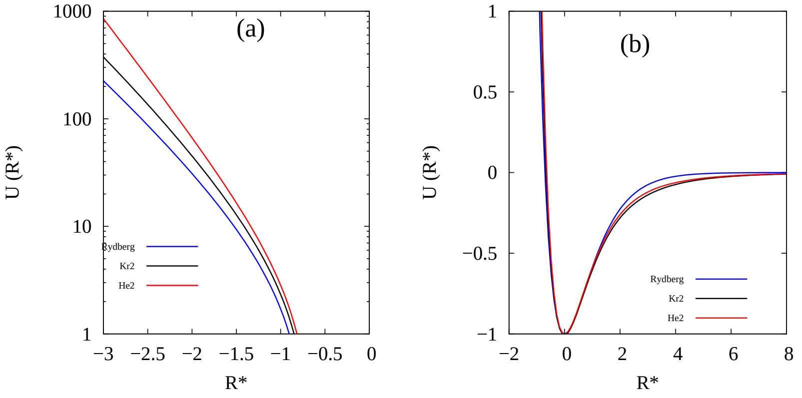

Fig.S11 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, Kr$_2$, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

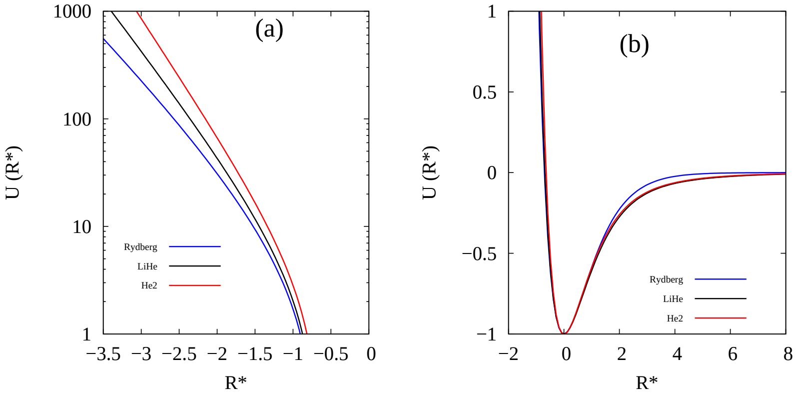

Fig.S12 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, LiHe, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

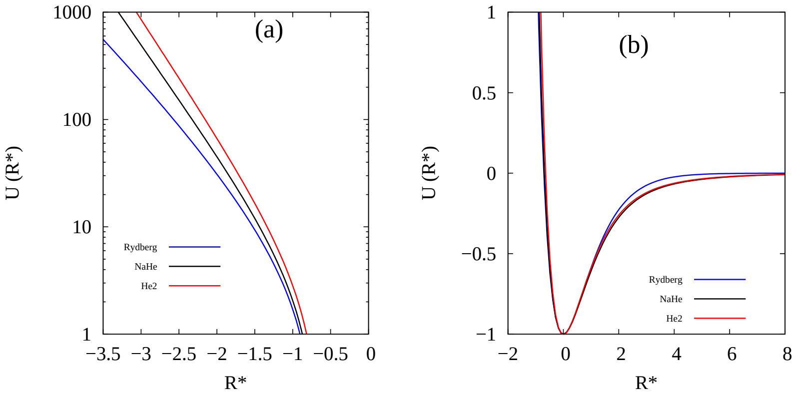

Fig.S13 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, NaHe, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

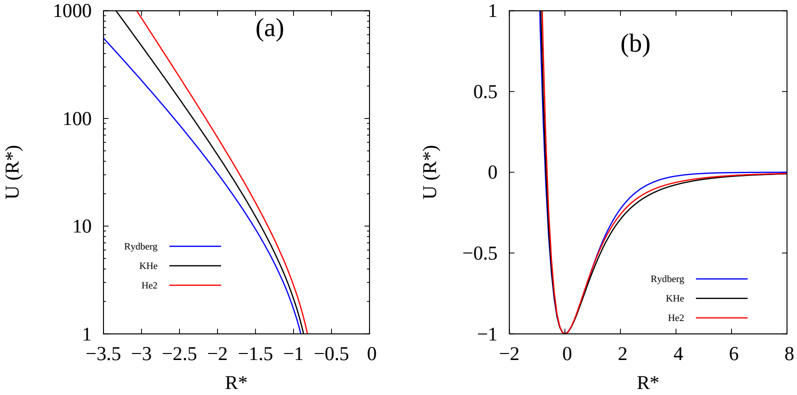

Fig.S14 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, KHe, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

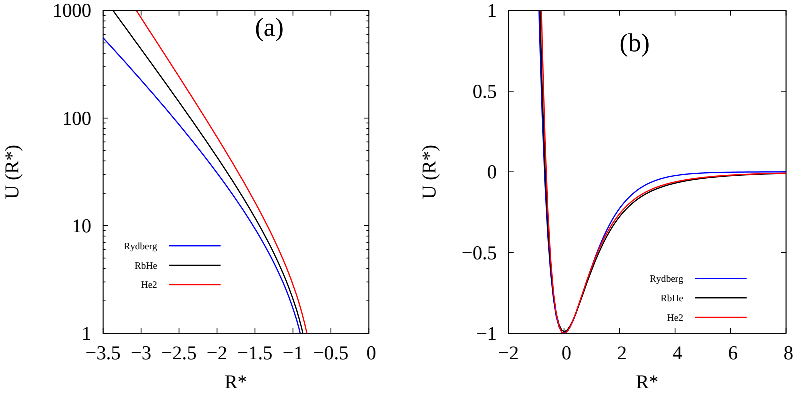

Fig.S15 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, RbHe, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

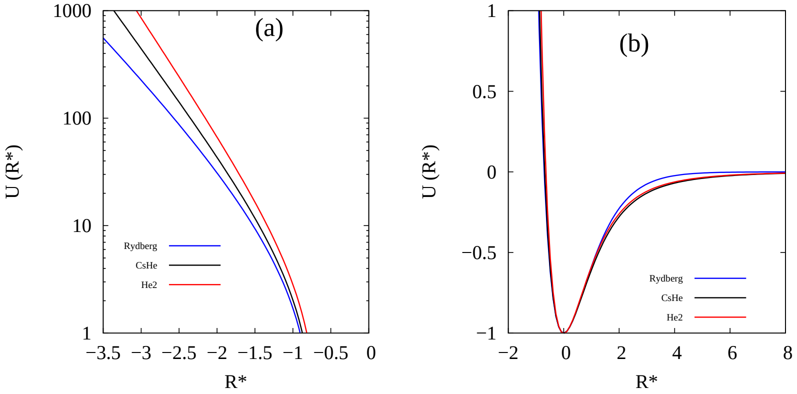

Fig.S16 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, CsHe, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

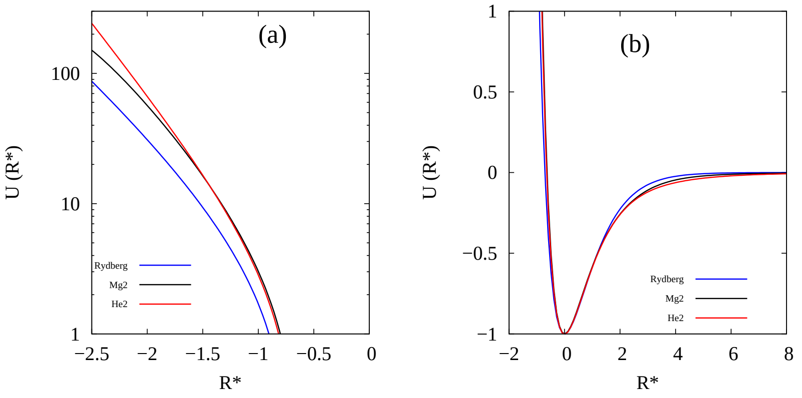

Fig.S17 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, Mg$_2$, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

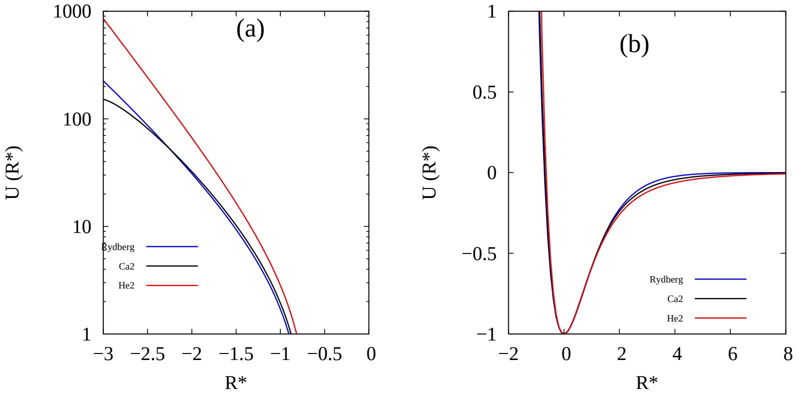

Fig.S18 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, Ca$_2$, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

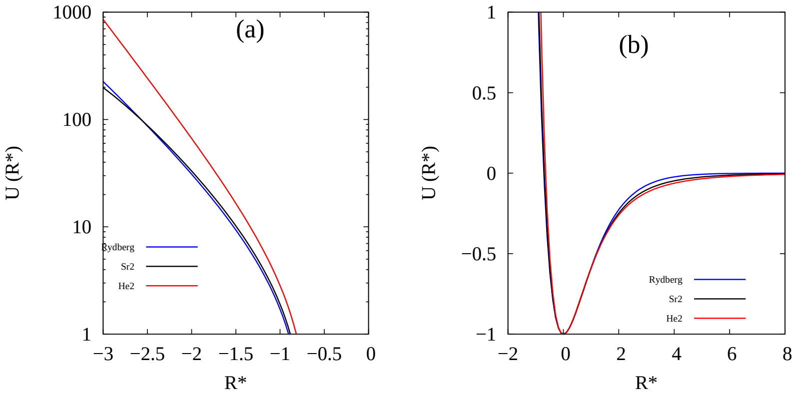

Fig.S19 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He$_2$, Sr$_2$, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

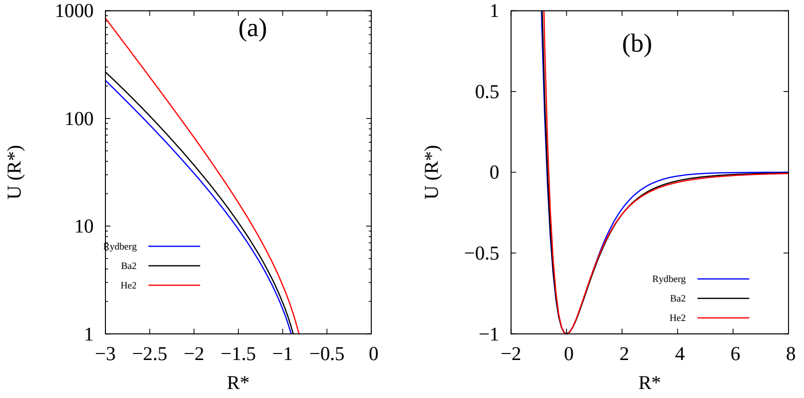

Fig.S20 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for $\mathrm{He_2}$, $\mathrm{Ba_2}$, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

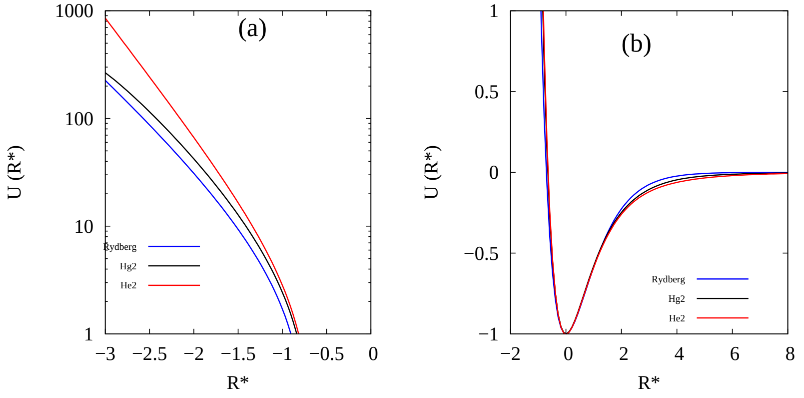

Fig.S21 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for $\mathrm{He_2}$, $\mathrm{Hg_2}$, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

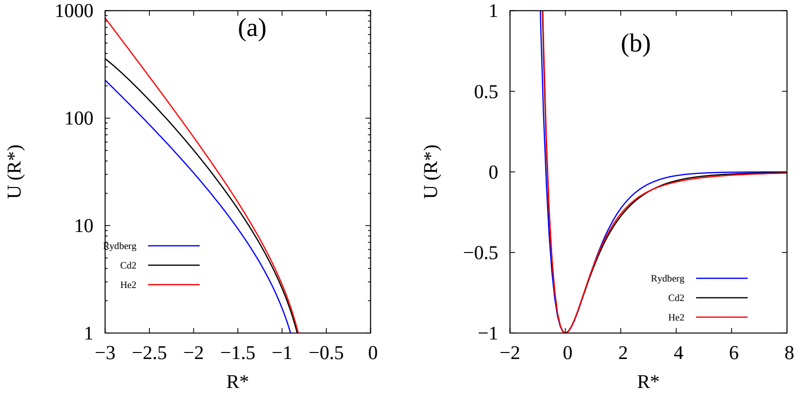

Fig.S22 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for $\mathrm{He_2}$, $\mathrm{Cd_2}$, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

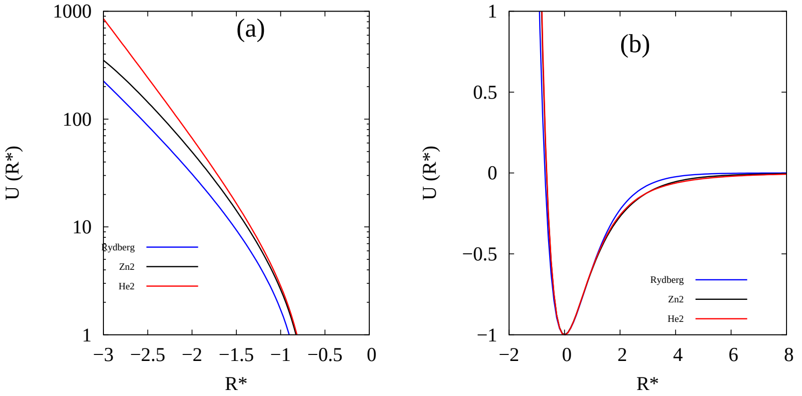

Fig.S23 Reduced potential curves $U(R^*) = V(R)/D_e$ ($V(R) = E(R) - E_\infty$, $D_e = |E_{min} - E_\infty|$) for He_2, Zn_2, and Rydberg function $U(R^*) = -(1 + \sqrt{2}R^*)e^{-\sqrt{2}R^*}$ with $R^* = (R - R_e)/L_2$.

7 How to Determine Potential Parameters?

Our purpose in this study is to provide a few-parameter analytical function form to uniformly describe the potential energy of diatomic systems. Here we present an approach to determine the potential parameters.

- **Step 1**: First, determine the parameters α, β, and γ in Eq.(1) following **Approach 1** (a simple Fortran code provided there) introduced in the supporting material of Ref. [23] (e.g., $\alpha = 1.313$, $\beta = 0.04200863$, $\gamma = 1.4$ for He_2 [23]);
- **Step 2**: Find the most accurate coefficients C_6, C_8 and C_{10} from the literature (e.g., $C_6 = 1.461$, $C_8 = 14.11$, and $C_{10} = 183.5$ for He_2 [5,8]). The higher-order coefficients C_{2n} ($n \geq 6$) can be derived by using the relation [5], $C_{2n} = (C_{2n-2}/C_{2n-4})^3 C_{2n-6}$. In this work, we set $n = 7$.
- **Step 3**: Determine the damping parameter ζ by setting $\zeta \approx 1.5R_e$ where R_e is the equilibrium distance ($R_e = 5.621$ Bohr [5,8,15,29] and $\zeta = 9$ for He_2).
- **Step 4**: Keep the γ value determined in Step 1 unchanged.
- **Step 5**: Adjust the parameter η in Eq.(2) starting from $\eta = 1$, tune the parameter α to adjust the equilibrium distance R_e, and tune the parameter β to adjust the well depth (for example, $\alpha = 1.41$, $\beta = 0.05056$, $\gamma = 1.4$, $\eta = 62.6$, and $\zeta = 9$ for He_2).

- **Step 6**: The above steps locate the range of the potential parameters. Then, use the Nonlinear Least-Square Fitting (NLLSF) Fortran program[1] that we provide in the supporting material to finally determine potential parameters α, β, γ, η, and ζ (In the Fortran program, we use He_2 as an example, and thus the input file for He_2 is provided also in the supporting material). To be noted, users may skip above Steps 1,3,4,5 and directly use NLLSF program to fit the potential to determine the potential parameter α, β, γ, η and ζ by setting the parameter range as follows: $\alpha = 0 \ \sim 5$, $\beta = 0 \sim 100$, $\gamma = 0 \ \sim 5$, $\eta = 0 \sim 100$, and $\zeta = 0 \sim 100$. In addition, users may use other NLLSF program that is available (For example, Matlab provides several functions for solving NLLSF problems).

The potential parameters determined for diatomic systems reported in this work are listed in Table 1.

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[1] To credit one of our authors, S. K. Mishra, who developed this program, cite the following reference: S. K. Mishra, "Performance of Differential Evolution Method in Least Squares Fitting of Some Typical Nonlinear Curves", Journal of Quantitative Economics, 5(1), 140-177 (2007).

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