Conformal Analytical Potential for All the Rare Gas Dimers over the Full Range of Internuclear Distances

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An analytical model for the potential between two rare gas atoms at distances between $R = 0$ to $R \to \infty$ is assumed to be conformal with the previously published potential for He$_2$ [J. Chem. Phys. **142**, 131102 (2015)]. The potential curves of the rare gas dimers all have the same shape and only depend on the well parameters D_e and R_e. The potentials and the vibrational levels for the 11 homonuclear and heteronuclear dimers for which recent *ab initio* calculations are available agree, within several percent, with the *ab initio* results. For the other rare gas dimers, the new potential provides the first realistic estimates for the potentials.

Born-Oppenheimer intermolecular potential energy curves (PEC) are fundamental for the microscopic understanding of the structure and the kinetic-dynamic behavior of atoms and molecules and their interactions in gases, liquids, and biological systems [1]. Experimental information on the PEC of small molecules can be obtained from transport property, molecular beam scattering and equation of state measurements, or laser spectroscopy of the molecules. The analysis relies on the analytical representations of the PEC, and the quality of the results depends on how realistic the chosen representation is. For systems consisting of many atoms, accurate PECs are calculated *ab initio* using modern electronic structure methods [2,3]. The weak van der Waals dispersive forces at long range, however, remain challenging [4]. The calculated *ab initio* energies can be used on the fly in the molecular dynamics simulations [5], but the costs are so high that the point-by-point energies are usually first fitted to a smooth analytic expression [6]. Here also the reliability of molecular dynamics or Monte Carlo simulations depends crucially on the accuracy of the underlying PEC. In the past, very complicated polynomial expansions with up to hundreds of parameters have been used [6]. Thus, in the analysis of both experiment and theory there is a need for accurate, faithful, analytic, physically motivated representations of PEC. Once an analytic formula is available, it can be used via molecular dynamics to predict many of the properties of the molecules and their collective behavior.

In the present contribution, a new 10 parameter model is introduced that provides an accurate generic description of potential energy curves between $R = 0$ to $R \to \infty$ of all 21 rare gas dimers with only two semiempirical parameters. The rare gas dimers are important prototype systems for developing potential models that properly account for the weak long range dispersive forces. The present analytic

representation is based on the established theories at the united atom limit and, at large internuclear distances, on the properly damped dispersion constants from theory. Because of its accuracy, the model provides an ideal representation for analyzing future experiments and an authentic basis for converting *ab initio* points into smooth curves for molecular dynamic calculations. The comparisons with the 11 dimers for which *ab initio* potential curves are available show good quantitative agreement. For the remaining 10 systems, the new model provides the first reliable estimates. With the new analytical potential, molecular dynamics simulations are now possible for the gas, liquid, and solid properties of the rare gases up to high pressures.

The new potential derives from an analytical potential, denoted TT2, for the helium dimer [7]. This potential, which was designed for the full range of internuclear distances from $R = 0$ to $R \to \infty$, consists of two terms, one for the short range repulsion and the other for the van der Waals region:

$$V_{\text{TT2}}(R) = V_{\text{short}}(R) + (1 - e^{-\alpha R})V_{\text{vdw}}(R), \qquad (1a)$$

where

$$V_{\text{short}}(R) = \frac{Z_A Z_B}{R}(1 + a_1 R + a_2 R^2 + a_3 R^3)e^{-\alpha R}, \qquad (1b)$$

$$V_{\text{vdw}}(R) = \Lambda R^{\frac{7}{\beta}-1} e^{-\beta R} - \sum_{n=3}^{5} \left[1 - e^{-bR} \sum_{k=0}^{2n} \frac{(bR)^k}{k!}\right] \frac{C_{2n}}{R^{2n}}. \qquad (1c)$$

The numerical values of the parameters in Eq. (1) for He$_2$, H$_2{}^3\sum_u^+$, and H-He$^2\sum^+$ are tabulated in Ref. [7]. The short range term $V_{\text{short}}(R)$ in Eq. (1b) is from the united atom

perturbation theory, where Z_A and Z_B are the nuclear charges of the separate atoms [8,9]. The energies of the separate atoms and the total energy of the united atom form the necessary boundary conditions at $R = 0$, which determine the rest of the parameters in the potential energy. In Eq. (1a), $V_{\text{short}}(R)$ replaces the van der Waals potential, which is turned off by the factor $[1 - \exp(-\alpha R)]$, where α is chosen such that R_e and D_e are not altered.

In Eq. (1c), the first term on the right is the Duman-Smirnov expression for the asymptotic exchange energy [10], where Λ depends sensitively on the amplitude of the wave function and $\beta = \sqrt{2\epsilon}$, with ϵ, the ionization energy. The second term is the long range attractive van der Waals potential, which is given by the London dispersion series [11] truncated at C_{10}, since the higher order terms are negligible [12]. Since the theory behind the dispersion coefficients is a well-defined problem [13], the coefficients can be accurately calculated [14,15]. The terms in the dispersion series are individually damped by the Tang and Toennies function given in the parenthesis in Eq. (1c) [16]. The potential representation Eq. (1c), denoted as TTY, was used in 1995 to determine the entire potential curve of the He dimer down to 3.00 a.u. [17] without any adjustable parameters. Recently, the TTY potential could be tested by comparison with a direct measurement of the wave function and the binding energy of the He dimer [18]. The well depth D_e and its location R_e predicted with the TTY formula [17], $D_e = 3.4789 \times 10^{-5}$ a.u. and $R_e = 5.615$ a.u., are in very good agreement with the latest values from experiment [19] and a very accurate recent *ab initio* calculation [20,21] that yields $D_e = 3.482 \times 10^{-5}$ a.u. and $R_e = 5.608$ a.u.. The expressions used here for the parameters Λ, β, and b in Eq. (1c) are derived in the Supplemental Material [22].

In the present context, Eq. (1) is written in the following reduced form:

$$V_{\text{TT2}}(R) = \frac{Z_A Z_B}{R_e} U_{\text{short}}(x) + D_e U_{\text{long}}(x), \qquad (2a)$$

where R_e and D_e are the well parameters and $x = R/R_e$. $Z_A Z_B / R_e$ is an energy in atomic units [22]. The $U_{\text{short}}(x)$ and $U_{\text{long}}(x)$ are reduced dimensionless potentials. We regard Eqs. (1) and (2) as a universal analytical potential model for van der Waals closed shell dimer systems.

In the present application of Eq. (1) to the rare gas dimers, the reduced potentials of Eq. (2a) are given by

$$U_{\text{short}}(x) = \frac{1}{x}(1 + a_1^* x + a_2^* x^2 + a_3^* x^3)e^{-\alpha^* x}$$

$$U_{\text{long}}(x) = (1 - e^{-\alpha^* x})U_{vdw}(x)$$

$$U_{\text{vdw}}(x) = A^* x^{\gamma^*} e^{-\beta^* x} - \sum_{n=3}^{5}\left[1 - e^{-b^* x}\sum_{k=0}^{2n}\frac{(b^* x)^k}{k!}\right]\frac{C_{2n}^*}{x^{2n}},$$

$$(2b)$$

TABLE I. Generic dimensionless parameters in Eq. (2b) for the rare gas dimers. The parameters $a_1, a_2 \dots$ for the He dimer are from Ref. [7]. The *ab initio* He dimer values used in the second column are $D_e(\text{He}_2) = 3.482 \times 10^{-5}$ and $R_e(\text{He}_2) = 5.608$ in a.u. [20].

Dimensionless parameter	Definition	Generic value
a_1^*	$a_1 R_e$	10.343
a_2^*	$a_2 R_e^2$	-23.687
a_3^*	$a_3 R_e^3$	12.343
α^*	αR_e	22.767
A^*	$\Lambda/D_e R_e^{(7/\beta)-1}$	45.612×10^5
γ^*	$(7/\beta) - 1$	1.531
β^*	βR_e	15.485
b^*	$b R_e$	13.950
C_6^*	$C_6/D_e R_e^6$	1.349 9
C_8^*	$C_8/D_e R_e^8$	0.414 7
C_{10}^*	$C_{10}/D_e R_e^{10}$	0.171 6

where the starred quantities are the *helium dimer* parameters of Eq. (1) reduced by the D_e and R_e of the helium dimer. The definition and the values of the starred dimensionless parameters are listed in Table I. The present Letter is based on the assumption that the potential model of Eq. (2a) and the He$_2$ starred parameters in Eq. (2b) are generic. They apply to all rare gas dimers with their specific R_e and D_e and Z_A and Z_B in Eq. (2a). In other words, it is assumed that all reduced potential curves, including the repulsive potentials of all rare gas dimers, have the same shape, i.e., are conformal with each other.

To test the model, the interatomic PECs of all 21 possible homogeneous and heterogeneous pairs of rare gas atoms are calculated with Eq. (2) and compared, where possible, to the results of recent *ab initio* calculations. The parameters $a_1^*, a_2^* \cdots$ in each case are the same and are equal to the generic values in Table I. The four essential parameters R_e, D_e, Z_A, and Z_B in Eq. (2) for each of the dimers are listed in Table II.

In Fig. 1, the PEC of He$_2$ from Ref. [7] from $R = 0$ a.u. over the full range of internuclear distances is compared to an *ab initio* quantum Monte Carlo calculation [34] and an *ab initio* investigation that included relativistic, adiabatic, and quantum electrodynamics effects [20,21]. Also shown is a united atom perturbation calculation that extends down to the united atom limit at $R = 0$ [35]. In the same figure, the present potential for Ar$_2$ is compared to three recent *ab initio* calculations [24,36,37]. Despite the fact that the well depth D_e of Ar$_2$ is some 13 times larger than that of He$_2$, on which Eq. (2) is based, the potential of Ar$_2$, with the same starred quantities, provides a similarly good fit as that of He$_2$.

In Fig. 2, the potentials of the other homogeneous rare gas dimers Ne$_2$, Kr$_2$, Xe$_2$, and Rn$_2$ are compared to *ab initio* results. Despite the large differences in the sizes of the atoms, the curves predicted by Eq. (2) closely follow the *ab initio* calculations. The same holds for the

TABLE II. Literature rare gas dimer potential well parameters R_e and D_e in a.u. and in, in parentheses, units of Å and ^0K, respectively. Z_A and Z_B are the nuclear charges of the atoms in a.u.

	Well location		Well depth			
	R_e	(R_e in Å)	$-D_e \times 10^5$	($-D_e$ in ^0K)	Z_A	Z_B
He-He	5.608 [a]	(2.97)	3.482 [a]	(10.99)	2	2
Ne-Ne	5.83 [b]	(3.09)	13.349 [b]	(42.15)	10	10
Ar-Ar	7.11 [c]	(3.76)	45.27 [c]	(142.95)	18	18
Kr-Kr	7.589 [d]	(4.02)	63.614 [d]	(200.87)	36	36
Xe-Xe	8.273 [e]	(4.38)	88.663 [e]	(279.97)	54	54
Rn-Rn	8.37 [f]	(4.43)	128.2 [f]	(404.81)	86	86
He-Ne	5.723 [g]	(3.03)	6.661 [g]	(21.03)	2	10
He-Ar	6.597 [h]	(3.49)	9.48 [h]	(29.93)	2	18
He-Kr	6.958 [i]	(3.68)	9.949 [i]	(31.42)	2	36
He-Xe	7.517 [j]	(3.98)	8.897 [j]	(28.09)	2	54
He-Rn	7.72 [k]	(4.09)	9.98 [k]	(31.51)	2	86
Ne-Ar	6.601 [g]	(3.49)	20.59 [g]	(65.02)	10	18
Ne-Kr	6.943 [l]	(3.67)	21.70 [l]	(68.52)	10	36
Ne-Xe	7.419 [m]	(3.93)	21.58 [m]	(68.14)	10	54
Ne-Rn	7.54 [k]	(3.99)	24.6 [k]	(77.68)	10	86
Ar-Kr	7.413 [l]	(3.92)	51.01 [l]	(161.07)	18	36
Ar-Xe	7.756 [m]	(4.10)	58.40 [m]	(184.41)	18	54
Ar-Rn	7.87 [k]	(4.16)	68.0 [k]	(214.72)	18	86
Kr-Xe	7.946 [m]	(4.20)	73.24 [m]	(231.27)	36	54
Kr-Rn	8.06 [k]	(4.27)	85.9 [k]	(271.24)	36	86
Xe-Rn	8.36 [k]	(4.42)	100.5 [k]	(317.35)	54	86

[a]Ref. [20].
[b]Ref. [23].
[c]Ref. [24].
[d]Ref. [25].
[e]Ref. [26].
[f]Ref. [27].
[g]Ref. [28].
[h]Ref. [29].
[i]Ref. [30].
[j]Ref. [31].
[k]Ref. [12].
[l]Ref. [32].
[m]Ref. [33].

FIG. 1. Potential curves of the ground state He$_2$ and Ar$_2$. The red lines are the present results. The points for He$_2$ are from Refs. [20,34,35]. The points for Ar$_2$ are from Refs. [24,36,37].

of Patkowski _et al._ for Ar$_2$ [24,36]. In the past, Ar$_2$ has served as an important prototype system for the development of reliable potentials between nonreactive systems. As seen in Fig. 1, the present Ar$_2$ potential closely follows, over 7

heterogeneous He-rare gas dimer potentials presented in Fig. 3(a) despite the large difference in the sizes of the rare gas atom compared to He. In Fig. 3(b),(c), the remainder of the rare gas interactions are compared to the available _ab initio_ calculations. For the 10 heavier rare gas dimers in Fig. 3 for which we have not found recent calculations, possibly because of relativistic effects [27], the present potential curves provide new accurate predictions for molecular dynamics calculations.

A more detailed comparison can be found in the Supplemental Material [22], where the difference between the present and _ab initio_ potentials is plotted as a function of the internuclear distance (Figs. S1 and S2). In the highly repulsive short-range region, there are few quantum chemical calculations and experimental results. The accuracy can only be based on comparisons to the coupled cluster calculations
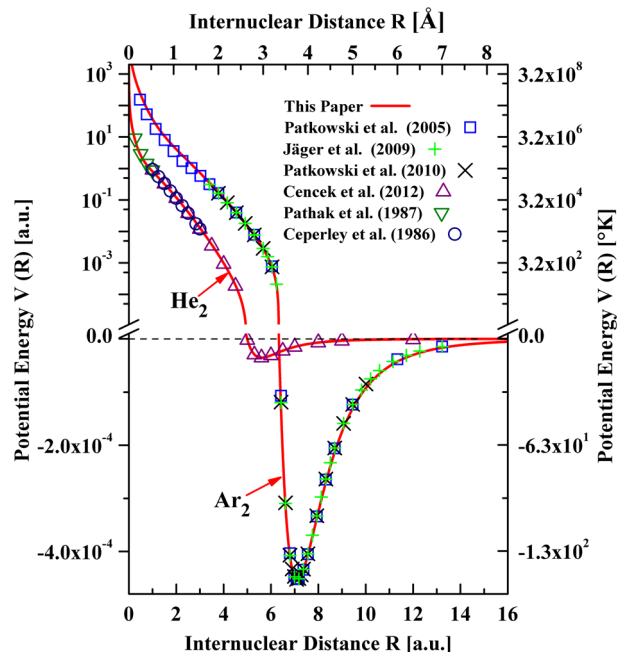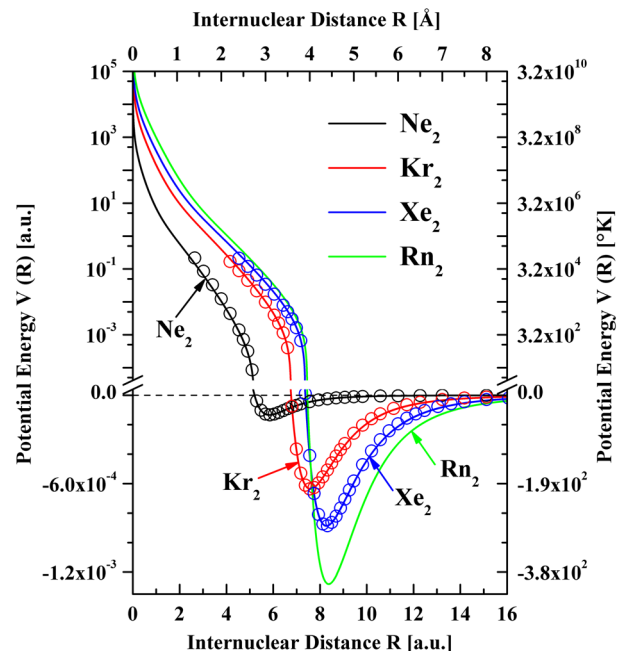

FIG. 2. Interatomic potential curves of the ground state Ne$_2$, Kr$_2$, Xe$_2$, and Rn$_2$. The black, red, blue, and green solid lines are the present predictions. The small black, red, and blue circles are the _ab initio_ results for the interaction potentials of Ne$_2$ [23], Kr$_2$ [25], and Xe$_2$ [26], respectively.
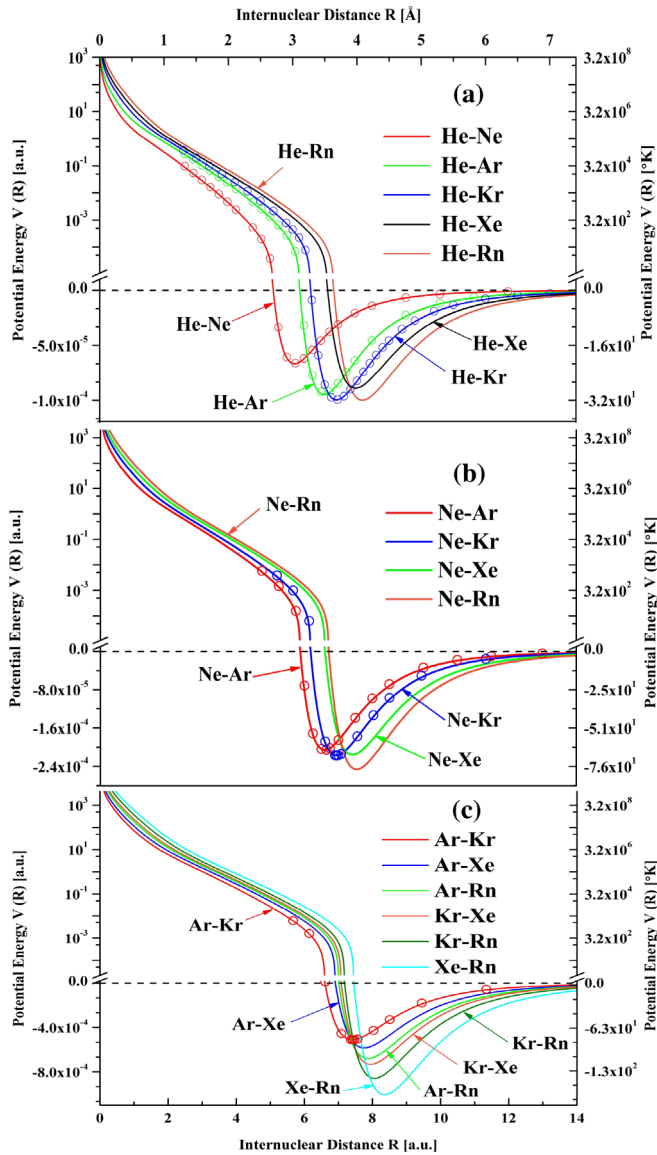
FIG. 3. Interatomic potential curves of the ground state hetero-nuclear rare gas dimers. The solid lines with different colors are the present predictions. The small circles are the *ab initio* results for the He-Ne [28], He-Ar [29], He-Kr [30], Ne-Ar [28], Ne-Kr [32], and Ar-Kr [32] potentials, respectively. (a) He-RGs (Ne, Ar, Kr, Xe, Rn). (b) Ne-RGs (Ar, Kr, Xe, Rn). (c) Ar-RGs (Kr, Xe, Rn), and Kr-RGs (Xe, Rn), and Xe-Rn.

orders of magnitude, the *ab initio* calculations. Only in the very highly repulsive region in the range of $R = 0.76$–2.3 a.u. the new potential is greater than the *ab initio* calculation by, on average, $+43\%$ [38]. The error then decreases until, at $R \geq 4.9$ a.u., corresponding to a repulsive energy of $V(R) \leq 5700$ K, it becomes less than 1%. Thus, at distances greater than about $R \geq 5$ a.u. the new potential agrees with the *ab initio* calculations within a percent.

Because of the conformality, the reduced second derivative at the minimum (force constant) and the third derivative (anharmonicity) are the same for all dimers and are $77.63 \pm$ 0.28 and -1561.56 ± 0.1, respectively. These values are surprisingly close to those of the Lennard-Jones (12,6) potential: 72 and -1512. Thus, it is not surprising that the vibrational levels calculated with the present potential listed in the Supplemental Material (Table S1, [22]) are in close agreement with the experimental and other theoretical results for the homonuclear dimers ($He_2 \sim Xe_2$) [39–45].

Compared to most previous models, the new potential curves cover the full range of internuclear distances from large distances down to the united atom limit $R = 0$. According to the law of corresponding states [46], the macroscopic thermodynamic properties V, P, and T of the heavier rare gases can be expressed in terms of D_e and R_e. With the new understanding on the conformality of the new potential between all pairs of rare gas atoms, the macroscopic properties of the rare gas atoms in the bulk gaseous, liquid, and solid states can be expected to be corresponding up to very high pressures.

It is, indeed, surprising that this universality can be modeled with an analytical potential originally developed to describe the He-He interaction. In many respects, the interactions with He are considered to be anomalous, e.g., no chemistry is known and it is the only substance that does not freeze at 0 K. Consequently, one of the important results of our work is the demonstration that all rare gas dimer potentials, including that of the He dimer, are conformal.

In view of the above demonstrated good performance of the new potential at small distances, it is ideal for simulations of the equation of state and the thermodynamic and elastic properties of the rare gas solids up to extreme pressures of several hundred GPa. At 500 GPa (500 Mbar) in solid argon, the smallest distances are about 4 to 5 a.u. where the potential is accurate to within several percent. The new potential provides a more realistic description than the Lennard-Jones and Buckingham potentials currently used in simulations of high pressure solids [47] and shock waves [48].

In conclusion, in this Letter a new generic analytical potential is introduced for all 21 dimer combinations of two rare gas atoms, including He_2, even for dimers with He and for the heaviest of the rare gas atoms, including Xe and Rn. Comparisons to *ab initio* calculations demonstrate that the new potential agrees, within several percent, with the potentials and vibrational levels of the homonuclear rare gas dimers. For the heavier dimers, for which older experimental estimates [12] but no recent *ab initio* calculations are available, the model potential provides new realistic potentials. Other than the nuclear charges, the potential only depends on the well depth D_e of the van der Waals minimum and its location R_e. The new potential is the first truly generic potential model for rare gas dimers over the entire range of internuclear distances.

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[22] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.125.253402 for a derivation of Eq. (2) and the parameters Λ, β, b, α, a_1, a_2, and a_3. There also curves are shown of the differences between the present potential and the available *ab initio* potentials. The vibrational levels of the homonuclear rare gas dimers ($He_2 \sim Xe_2$) are tabulated and compared to experimental and other theoretical data.

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