

# Application of Maclaurin series in relating interatomic potential functions: A review

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This paper provides a short review on the application of Maclaurin series in relating potential functions within the same category of interatomic interaction. The potential functions covered are those commonly adopted in computational chemistry softwares. While various mathematical approaches have been employed in generating relationships amongst potential functions, the use of Maclaurin series has been prevalent recently due to the increasing application of polynomial series-type potential functions. In the case of covalent bond-stretching, the Maclaurin series for the exponential function is used to transform the Morse potential into the polynomial series potential, and vice versa. For covalent bond-bending, Maclaurin series for the sine and cosine functions were employed to extract polynomial angle series potential from the Fourier series and harmonic cosine potential functions, and vice versa. Finally, both the exponential and the  $1/(1-x)$  expressions in Maclaurin series were used in obtaining the exact relationship for the repulsive terms between two potential functions.

**KEY WORDS:** Interatomic interaction, Maclaurin series, polynomial functionals, potential function

**AMS subject classification:** 11C08, 26C99, 30B10, 41A10, 74A25, 81V55

## Nomenclature

The symbols adopted in this paper for interatomic potential function parameters follow the meaning given in this list, unless otherwise stated.

$\alpha$	shape parameter of Morse potential
$A$	magnitude parameter of repulsion energy in exponential-6 potential
$B$	shape parameter of repulsion energy in exponential-6 potential
$C$	parameter of attractive energy in exponential-6 potential
$C_n$	Fourier series shape parameter
$D_M$	bond dissociation energy in Morse potential
$D_{9-6}^{LJ}$	magnitude of minimum well-depth in Lennard-Jones (9-6) potential

$D_{12-6}^{\text{LJ}}$	magnitude of minimum well-depth in Lennard–Jones (12–6) potential
$\eta$	order of accuracy from exponential-6 to Lennard–Jones potentials
$k^{(n)}$	correction factor for repulsive energy between exponential-6 and Lennard–Jones
$k_{\text{C}}$	harmonic cosine stiffness parameter
$k_{\text{F}}$	Fourier series “stiffness” ( $n = 0, 1, 2$ )
$k_{\text{H}}$	harmonic parameter (Hookean stiffness)
$k_{\text{S}_n}$	polynomial series parameters ( $n = 1, 2, 3, \dots$ )
$k_{\theta}$	harmonic angle parameter (angular stiffness)
$k_{\theta_n}$	polynomial angle series parameter ( $n = 1, 2, 3, \dots$ )
$r$	bond length for covalent bonds or interatomic distance for non-bonds
$r_0$	equilibrium bond length
$R$	van der Waals equilibrium distance for non-bonds
$\theta$	bond angle
$\theta_0$	equilibrium bond angle
$U_{\text{C}}$	harmonic cosine potential energy
$U_{\text{F}}$	Fourier series potential energy
$U_{\text{H}}$	harmonic potential energy
$U_{9-6}^{\text{LJ}}$	Lennard–Jones (9–6) potential energy
$U_{12-6}^{\text{LJ}}$	Lennard–Jones (12–6) potential energy
$U_{\text{M}}$	Morse potential energy
$U_{\text{S}}$	polynomial series potential energy
$U_{\text{S}\theta}$	polynomial angle series potential energy
$U_{\theta}$	harmonic angle potential energy
$U_{\text{X}6}$	exponential-6 potential energy
$\xi$	scaling factor between exponential-6 and Lennard–Jones potential functions

## 1. Introduction

Although chemistry is largely concerned with reactions whereby chemical bonds are broken and reformed, the interatomic forces between unreacting atoms and molecules are nonetheless of great significance. In chemical/molecular and nano-scale sciences, molecular-scale objects that are being investigated are of extremely low dimension that direct experimental observation and/or measurement is difficult, costly and hindered by instrument limitations. As a result, computer modeling and simulation now play a vital role in the molecular sciences and related fields. Interatomic potential functions are essential in quantifying the molecular system energies, and are adopted in computational chemistry softwares. For further development of these interatomic interactions, researchers have turned to mathematical approaches for gaining insight into fundamental knowledge and possible applications (e.g., [1–17]). Recently a number

of relationships between empirical potential functions of the same class of interatomic interactions were developed [18–26] for the purpose of developing a molecular potential function converter. In most of these potential function relationships, the Maclaurin series expansions have been widely used in extracting the polynomial functional forms from the “more realistic” potential functions. Conversely a given polynomial-type potential function can be inverted to give other potential functions within the same category of interatomic interaction [27]. The Maclaurin series were also employed in obtaining a spectrum of van der Waals curves—ranging from the purely Exponential-6 to the purely Lennard–Jones potential functions. A browse through table 1 shows a balanced adoption of polynomial-type and non-polynomial-type potential functions for 2-body and 3-body interactions, thereby underlining the importance of parametric conversions amongst these potential functions [28–46]. Likewise the balanced distribution among Exponential-6 and Lennard–Jones type of van der waals potentials (see table 1) underscores the relevance of exact relationship between their parameters. This paper gives a review on the application of Maclaurin series in relating the interatomic potential functions with particular focus on the reasoning and strategy involved.

## 2. Maclaurin series

The application of polynomials in mathematical chemistry is nothing new. For example, the Gegenbauer polynomials have been used to calculate the multi-center nuclear attraction and electron repulsion integrals over Slater orbitals by Fourier transform method [47]. In the case of “Maclaurin-based” polynomials, we first consider the Taylor series expansion:

$$f(x) = \sum_{n=0}^{\infty} f^{(n)}(x_0) \frac{(x - x_0)^n}{n!} = f(x_0) + f'(x_0) \frac{(x - x_0)}{1!} + f''(x_0) \frac{(x - x_0)^2}{2!} + \dots \quad (1)$$

The generalized Maclaurin series expansion is the special case of equation (1) whereby  $x_0 = 0$

$$f(x) = \sum_{n=0}^{\infty} f^{(n)}(0) \frac{x^n}{n!} = f(x_0) + f'(x_0) \frac{x}{1!} + f''(x_0) \frac{x^2}{2!} + \dots \quad (2)$$

A list of some simple Maclaurin series are furnished in the appendix. Of these, equations (A1) and (A4)–(A6) have been employed in relating interatomic potential functions that are used in computational chemistry softwares. The following sections review the applications of specific Maclaurin series expansions in generating polynomial functionals based on other potential functions of the same category of interatomic interaction, and extraction of the latter functions from the polynomial forms.

Table 1

Comparison of potential functions used in some computational chemistry softwares, arranged in chronological order (m refers to the order of the polynomial-type potential functions).

Comput. Chem. software	2-Body (polynomial-type)	2-Body (other types)	3-Body (polynomial-type)	3-Body (other types)	van der Waals	Ref.
EAS		Harmonic	$m = 3$	Harmonic	X6	[28]
MM2	$m = 3$	Harmonic and Morse	$m = 6$	Harmonic	X6	[29]
CVFF				Harmonic	LJ(12-6)	[30]
CHARMM		Harmonic		Harmonic	LJ(12-6)	[31]
GROMOS		Harmonic		Harmonic	LJ(12-6)	[32]
TRIPOS		Harmonic		Harmonic	LJ(12-6)	[33]
MM3	$m = 4$	Harmonic and Morse	$m = 6$	Harmonic	X6	[34]
DREIDING		Harmonic and Morse		Harmonic cosine	X6 and LJ(12-6)	[35]
COSMIC		Harmonic		Harmonic	Morse	[36]
SHAPES		Harmonic		Fourier	LJ(12-6)	[37]
UFF		Harmonic and Morse		Fourier	LJ(12-6)	[38]
CFF	$m = 4$	Harmonic	$m = 4$	Harmonic	LJ(9-6)	[39]
AMBER					LJ(12-6) and LJ(12-10)	[40]
MOMECC		Harmonic		Harmonic	X6	[41]
EFF	$m = 4$	Harmonic	$m = 3$	Harmonic	X6	[42]
ESFF		Morse		Harmonic cosine	LJ(9-6)	[43]
MMFF	$m = 4$	Harmonic	$m = 3$		LJ(14-7)	[44]
MM4	$m = 6$		$m = 6$		X6	[45]
OPLS		Harmonic		Harmonic	LJ(12-6)	[46]

### 3. Application in bond-stretching potentials

The simplest relation among parameters of bond-stretching potentials is that between the harmonic potential:

$$U_H = \frac{1}{2}k_H(r - r_0)^2 = \frac{1}{2}k_H(\delta r)^2 \quad (3)$$

and the Morse potential

$$U_M = D_M \{1 - \exp[-\alpha(r - r_0)]\}^2. \quad (4)$$

By equating

$$\left. \frac{\partial^2 U_H}{\partial r^2} \right|_{r=r_0} = \left. \frac{\partial^2 U_M}{\partial r^2} \right|_{r=r_0}, \quad (5)$$

we have

$$k_H = 2D_M\alpha^2. \quad (6)$$

Here we note that the harmonic parameter can be obtained from Morse parameters but not vice versa. The third type of 2-body potential function is an extension of the harmonic potential, also known as the polynomial series potential function:

$$U_S = \frac{1}{2} \sum_{n=2}^m k_{S_n} (\delta r)^n, \quad (7)$$

whereby  $m$  is a positive integer greater than  $n$ . By substituting equation (A4) into equation (4), and arranging the terms in a series of increasing order of  $(\delta r)$ , we obtain the following potential energy description:

$$\frac{U_M}{D_M} = \alpha^2(\delta r)^2 - \alpha^3(\delta r)^3 + \frac{7}{12}\alpha^4(\delta r)^4 - \frac{1}{4}\alpha^5(\delta r)^5 + \frac{31}{360}\alpha^6(\delta r)^6 - \dots \quad (8)$$

By neglecting all except the first term, we have

$$U_M = D_M\alpha^2(\delta r)^2, \quad (9)$$

which, upon comparison with equation (3), gives equation (6). The latter approach, however, is more than just an alternative approach. By considering the first three terms of equation (8), we arrive at

$$U_M = D_M\alpha^2(\delta r)^2 \left[ 1 - \alpha(\delta r) + \frac{7}{12}\alpha^2(\delta r)^2 \right]. \quad (10)$$

Equation (10) was reported in the late 1980s by Allinger et al. [34], with credit given to one Professor L.S. Bartell. Although no mathematical proof was furnished (to this author's knowledge), the exactness in the fractional form reveals the usage of series expansion. By comparing terms of equations (7) and (8), we have

$$\begin{Bmatrix} k_{S_2} \\ k_{S_3} \\ k_{S_4} \\ k_{S_5} \\ k_{S_6} \end{Bmatrix} = 2D_M\alpha^2 \begin{Bmatrix} 1 \\ -\alpha \\ (7/12)\alpha^2 \\ -(1/4)\alpha^3 \\ (31/360)\alpha^4 \end{Bmatrix}. \quad (11)$$

Whilst a given harmonic potential cannot be converted into a Morse potential, such conversion is possible for a given polynomial series potential function. Solving the first two rows of equation (11) gives the Morse parameters in terms of the polynomial series parameters [24, 27]:

$$\alpha = -\frac{k_{S_3}}{k_{S_2}}, \quad (12)$$

$$D_M = \frac{k_{S_2}^3}{2k_{S_3}^2}. \quad (13)$$

Alternatively, solving the first and third rows of equation (11) leads to

$$\alpha = \sqrt{\frac{12}{7} \left( \frac{k_{S_4}}{k_{S_2}} \right)}, \quad (14)$$

$$D_M = \frac{7}{24} \left( \frac{k_{S_2}^2}{k_{S_4}} \right). \quad (15)$$

The trend goes on whereby any combination of two  $k_{S_n}$  parameters can give the two Morse parameters. This is hardly surprising since it is easy to see that two independent equations are required to solve for two variables. In a parallel development [48], both equations (A1) and (A4) were applied to obtain a long range relationship between the Morse potential and the Rydberg potential [49] (also known as the 2-body portion of Murrell-Mottram potential [50]).

#### 4. Application in bond-bending potentials

Commonly adopted potential functions for 3-body interactions are the harmonic angle potential

$$U_\theta = \frac{1}{2}k_\theta (\theta - \theta_0)^2 = \frac{1}{2}k_\theta (\delta\theta)^2, \quad (16)$$

the polynomial angle series potential

$$U_{S_\theta} = \frac{1}{2} \sum_{n=2}^m k_{\theta_n} (\delta\theta)^n, \quad (17)$$

the Fourier series potential

$$U_F = k_F \sum_{n=0}^m C_n \cos(n\theta) \quad (18)$$

and the harmonic cosine potential

$$U_C = \frac{1}{2} k_C (\cos\theta - \cos\theta_0)^2. \quad (19)$$

To apply the Maclaurin series expansions, we firstly express the bond angle ( $\theta$ ) in terms of the equilibrium bond angle ( $\theta_0$ ) and the amount of bending ( $\delta\theta$ ):

$$\theta = \theta_0 + \delta\theta. \quad (20)$$

To do so in transforming the harmonic cosine parameters to polynomial angle series parameters, it is essential that the following term in equation (19) be expanded as

$$\begin{aligned} (\cos\theta - \cos\theta_0)^2 &= \cos^2\theta_0 [\cos^2(\delta\theta) - 2\cos(\delta\theta) + 1] \\ &\quad + 2\sin\theta_0 \cos\theta_0 \sin(\delta\theta) [1 - \cos(\delta\theta)] + \sin^2\theta_0 \sin^2(\delta\theta). \end{aligned} \quad (21)$$

Substituting the Maclaurin series expansions, equations (A5) and (A6), into the terms  $\cos(\delta\theta)$  and  $\sin(\delta\theta)$ , respectively in equation (21), and rearranging in increasing powers of ( $\delta\theta$ ), we arrive at [19]

$$\begin{aligned} U_C &= \frac{1}{2} k_C \sin^2\theta_0 (\delta\theta)^2 + \frac{1}{2} k_C \sin\theta_0 \cos\theta_0 (\delta\theta)^3 \\ &\quad - \frac{1}{2} k_C \left( \frac{1}{3} \sin^2\theta_0 - \frac{1}{4} \cos^2\theta_0 \right) (\delta\theta)^4 - \frac{1}{2} k_C \left( \frac{1}{4} \sin\theta_0 \cos\theta_0 \right) (\delta\theta)^5 \\ &\quad + \frac{1}{2} k_C \left( \frac{2}{45} \sin^2\theta_0 - \frac{1}{24} \cos^2\theta_0 \right) (\delta\theta)^6. \end{aligned} \quad (22)$$

Comparing equation (22) with equation (17) for  $m = 6$  gives the polynomial angle parameters in terms of harmonic cosine parameters

$$\begin{Bmatrix} k_{\theta_2} \\ k_{\theta_3} \\ k_{\theta_4} \\ k_{\theta_5} \\ k_{\theta_6} \end{Bmatrix} = k_C \begin{Bmatrix} \sin^2\theta_0 \\ \sin\theta_0 \cos\theta_0 \\ -(1/3) \sin^2\theta_0 + (1/4) \cos^2\theta_0 \\ -(1/4) \sin\theta_0 \cos\theta_0 \\ (2/45) \sin^2\theta_0 - (1/24) \cos^2\theta_0 \end{Bmatrix}. \quad (23)$$

By solving the first two rows of equation (23), we have the harmonic cosine parameter in terms of the polynomial angle parameters [24, 27]:

$$k_C = \frac{2(k_{\theta_2} - k_{\theta_3})}{1 - (\sin 2\theta_0 + \cos 2\theta_0)}. \quad (24)$$

A simpler alternative would be the use of the first and third rows of equation (23), which gives

$$k_C = \frac{4}{3} \left( \frac{k_{\theta_2} + k_{\theta_4}}{\cos^2 \theta_0} \right). \quad (25)$$

As in the case of obtaining Morse parameters in 2-body interaction, any combination of two  $k_{\theta_n}$  parameters – with the equilibrium bond angle  $\theta_0$  – can lead to the harmonic cosine stiffness parameter,  $k_C$ .

In relating the Fourier series parameters to the polynomial angle series parameter, it is essential to apply equation (20) in equation (18) such that

$$\sum_{n=0}^2 C_n \cos(n\theta) = \sum_{n=0}^2 C_n [\cos(n\theta_0) \cos(n\delta\theta) - \sin(n\theta_0) \sin(n\delta\theta)]. \quad (26)$$

Substituting the Maclaurin series expansions – i.e. equations (A5) and (A6) into the terms  $\cos(\delta\theta)$  and  $\sin(\delta\theta)$ , respectively in equation (26) – and arranging in increasing powers of  $\delta\theta$  leads to [19]

$$\begin{aligned} U_F &= k_F (C_0 + C_1 \cos \theta_0 + C_2 \cos 2\theta_0) - k_F (C_1 \sin \theta_0 + 2C_2 \sin 2\theta_0) (\delta\theta) \\ &\quad - \frac{1}{2} k_F (C_1 \cos \theta_0 + 4C_2 \cos 2\theta_0) (\delta\theta)^2 + \frac{1}{6} k_F (C_1 \sin \theta_0 + 8C_2 \sin 2\theta_0) (\delta\theta)^3 \\ &\quad + \frac{1}{24} k_F (C_1 \cos \theta_0 + 16C_2 \cos 2\theta_0) (\delta\theta)^4 \\ &\quad - \frac{1}{120} k_F (C_1 \sin \theta_0 + 32C_2 \sin 2\theta_0) (\delta\theta)^5 \\ &\quad - \frac{1}{720} k_F (C_1 \cos \theta_0 + 64C_2 \cos 2\theta_0) (\delta\theta)^6 \end{aligned} \quad (27)$$

or, in a more compact form,

$$\begin{aligned} \frac{U_F}{k_F} &= \sum_{p=0}^3 \sum_{n=0}^2 \frac{(-1)^p}{(2p)!} n^{2p} C_n \cos(n\theta_0) (\delta\theta)^{2p} \\ &\quad + \sum_{p=1}^3 \sum_{n=0}^2 \frac{(-1)^p}{(2p-1)!} n^{2p-1} C_n \cos(n\theta_0) (\delta\theta)^{2p-1}. \end{aligned} \quad (28)$$



Comparing equation (27) with equation (17) for  $m = 6$  yields the polynomial angle parameters in terms of Fourier series parameters:

$$\begin{Bmatrix} k_{\theta_2} \\ k_{\theta_3} \\ k_{\theta_4} \\ k_{\theta_5} \\ k_{\theta_6} \end{Bmatrix} = 2k_F \begin{Bmatrix} -\frac{1}{2!} \sum_{n=1}^2 n^2 C_n \cos(n\theta_0) \\ +\frac{1}{3!} \sum_{n=1}^2 n^3 C_n \sin(n\theta_0) \\ +\frac{1}{4!} \sum_{n=1}^2 n^4 C_n \cos(n\theta_0) \\ -\frac{1}{5!} \sum_{n=1}^2 n^5 C_n \sin(n\theta_0) \\ -\frac{1}{6!} \sum_{n=1}^2 n^6 C_n \cos(n\theta_0) \end{Bmatrix}, \tag{29}$$

with the implication that the first two terms of equation (27) are zero, i.e.,

$$k_{\theta_0} = 2k_F \sum_{n=0}^2 C_n \cos(n\theta_0) = 0, \tag{30}$$

$$k_{\theta_1} = -2k_F \sum_{n=0}^2 n C_n \sin(n\theta_0) = 0. \tag{31}$$

Indeed, solving for  $C_n (n = 0, 1, 2)$  from equations (30) and (31) simultaneously gives the solution by Rappe et al. [38]:

$$C_0 = C_2(2 \cos^2 \theta_0 + 1), \tag{32}$$

$$C_1 = -4C_2 \cos \theta_0, \tag{33}$$

$$C_2 = \frac{1}{4 \sin^2 \theta_0}. \tag{34}$$

However, the Fourier series furnished in equation (29) is expressed in terms of  $k_F, C_n (n = 0, 1, 2)$  and  $\theta$ , but not in terms of  $\theta_0$ . Nevertheless it can be easily seen from equations (33) and (34) that

$$\cos \theta_0 = -\frac{1}{4} \left( \frac{C_1}{C_2} \right) \tag{35}$$

and

$$\sin \theta_0 = \frac{1}{2\sqrt{C_2}}, \tag{36}$$

thus enabling the term  $\theta_0$  to be eliminated from equation (29). This gives

$$\begin{Bmatrix} k_{\theta_2} \\ k_{\theta_3} \\ k_{\theta_4} \\ k_{\theta_5} \\ k_{\theta_6} \end{Bmatrix} = k_F \begin{Bmatrix} 1 \\ -(1/2)(C_1/\sqrt{C_2}) \\ -(4/3)C_2 [1 - (7/64)(C_1/C_2)^2] \\ (1/8)(C_1/\sqrt{C_2}) \\ (8/45)C_2 [1 - (31/156)(C_1/C_2)^2] \end{Bmatrix}, \quad (37)$$

which expresses the polynomial angle parameters in purely Fourier series parameters. Conversely, one may obtain the Fourier series from a given polynomial angle potential function. The first row of equation (37) simply reveals that

$$k_F = k_{\theta_2}. \quad (38)$$

Note that equation (29), which is the equivalent form of equation (37), gives no such salient indication. The other parameter from the polynomial series potential,  $\theta_0$ , simply leads to the values of  $C_n$  ( $n = 0, 1, 2$ ), as evident from equations (32)–(34). That the extraction of Fourier series parameters can be made without solving from any two rows from equation (37) is obvious, since equation (37) is obtained with the aid of equations (32)–(34), in the first instance.

## 5. Application in van der Waals potentials

Development of a mathematical relationship between the exponential-6

$$U_{X6} = A \exp(-Br) - \frac{C}{r^6} \quad (39)$$

and the generalized Lennard–Jones ( $m-n$ ) potential

$$U_{m-n}^{\text{LJ}} = D_{m-n}^{\text{LJ}} \left[ \frac{n}{m-n} \left( \frac{R}{r} \right)^m - \frac{m}{m-n} \left( \frac{R}{r} \right)^n \right]; \quad m > n \quad (40)$$

has been attempted, shown to be applicable for  $n = 6$ , and illustrated for the common cases of Lennard–Jones (12–6) and Lennard–Jones (9–6) potential functions [21]. While relationship between the Lennard–Jones ( $m-6$ ), for  $m > 6$ , and the exponential-6 potential functions has been shown to be exact for the case of near equilibrium, a discrepancy was observed for the case of long-range relationship in the repulsive term. That is, the loose form of the Exponential-6 potential

$$U_{X6} = D_{m-6}^{\text{LJ}} \left\{ \frac{6}{\xi-6} \exp \left[ \xi \left( 1 - \frac{r}{R} \right) \right] - \frac{\xi}{\xi-6} \left( \frac{R}{r} \right)^6 \right\} \quad (41)$$

has been shown to be faulty in the repulsive part of equation (41) which, upon comparing with that of equation (40) for  $m = 2n = 12$ , incorrectly implies that

$$\frac{R}{r} = \exp \left( 1 - \frac{r}{R} \right). \quad (42)$$

As a result of this error the loose form of exponential-6 function described by equation (41) gives a finite value at  $r = 0$ , just as its original form as shown in equation (39) would, whilst the Lennard–Jones functions give infinite value. To deal with this error a correction factor  $k$ , raised to the power of  $\xi$ , was introduced into the repulsive term in equation (41) such that

$$U_{X6}^{(\eta)} = D_{m-6}^{LJ} \left\{ (k^{(\eta)})^{\xi} \frac{6}{\xi - 6} \exp \left[ \xi \left( 1 - \frac{r}{R} \right) \right] - \frac{\xi}{\xi - 6} \left( \frac{R}{r} \right)^6 \right\}, \quad (43)$$

where  $\eta$  refers to the order of accuracy. This order of accuracy is a measure of the extent to which the loose form of Exponential-6 conforms to the Lennard–Jones form. Comparison between equations (40) and (43) for  $m = \xi = 2n = 12$  gives

$$\frac{R}{r} = k^{(\eta)} \exp \left( 1 - \frac{r}{R} \right). \quad (44)$$

As such, applying the Maclaurin series of equations (A1) and (A4), we have

$$\exp \left( 1 - \frac{r}{R} \right) = \exp \left( -\frac{\delta r}{R} \right) \equiv \sum_{\eta=0}^{\infty} \frac{1}{\eta!} \left( -\frac{\delta r}{R} \right)^{\eta} \quad (45)$$

and

$$\frac{R}{r} = \frac{1}{1 - (-\delta r/R)} \equiv \sum_{\eta=0}^{\infty} \left( -\frac{\delta r}{R} \right)^{\eta}, \quad (46)$$

respectively. Substituting the Maclaurin series expressions of equations (45) and (46) into equation (44) gives the correction factor

$$k^{(\eta)} = \frac{\sum_{i=0}^{\eta} (-\delta r/R)^i}{\sum_{i=0}^{\eta} (-\delta r/R)^i / i!}. \quad (47)$$

A limiting case of the correction factor is where  $k = 1$  (or when the order of accuracy  $\eta = 0$ ), that corresponds to a purely exponential-6 form. On the other hand as  $\eta \rightarrow \infty$  equation (43) tends towards the other end of the spectrum, which constitutes the purely Lennard–Jones form. As such, for any positive integer of the order of accuracy within  $0 < \eta < \infty$ , we encounter the case of an interlace between exponential-6 and Lennard–Jones forms. Since the factor  $(k^{(\eta)})^{\xi}$  occurs at the repulsive term, the correction factor enables a more flexible curve-fitting at the repulsive region ( $0 < r < R$ ) without interfering with the curve-fitting on the attractive region ( $R < r < \infty$ ).

## 6. Closure

Relating potential functions is a necessity when a mismatch occurs between available reliable parametric data and the computational chemistry softwares' potential functions. Recent publication on the applications and the extent of applicability of Maclaurin series expansions for relating interatomic potential functions have been reviewed in this paper. The choice of Maclaurin series is a natural one since they enable the expansion of functions into power series, thereby allowing comparison of terms with the polynomial-type potential functions.

### Appendix: A list of some Maclaurin series expansions

$$\frac{1}{1-x} = 1 + x^1 + x^2 + x^3 + \dots \quad \text{for } -1 < x < 1, \quad (\text{A1})$$

$$\ln(1+x) = \frac{x^1}{1} - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \dots \quad \text{for } -1 < x < 1, \quad (\text{A2})$$

$$\frac{1}{2} \ln \left( \frac{1+x}{1-x} \right) = \frac{x^1}{1} - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \dots \quad \text{for } -1 < x < 1, \quad (\text{A3})$$

$$\exp x = 1 + \frac{x^1}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots, \quad (\text{A4})$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots, \quad (\text{A5})$$

$$\sin x = \frac{x^1}{1!} - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots, \quad (\text{A6})$$

$$\tan x = x + \frac{1}{3}x^3 + \frac{2}{15}x^5 + \frac{17}{315}x^7 + \dots, \quad (\text{A7})$$

$$\sec x = 1 + \frac{1}{2!}x^2 + \frac{5}{4!}x^4 + \frac{61}{6!}x^6 + \dots, \quad (\text{A8})$$

$$\csc x = \frac{1}{1}x^{-1} + \frac{1}{6}x^1 + \frac{7}{360}x^3 + \frac{31}{15120}x^5 + \dots, \quad (\text{A9})$$

$$\cot x = \frac{1}{1}x^{-1} - \frac{1}{3}x^1 - \frac{1}{45}x^3 - \frac{2}{945}x^5 - \dots \quad (\text{A10})$$

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