

# Electronic Supplementary Information

## An analytical expression for the van der Waals interaction in oriented-attachment growth: a spherical nanoparticle and a growing cylindrical nanorod

Weidong He <sup>†‡</sup>, Junhao Lin <sup>‡||</sup>, Bin Wang <sup>||</sup>, Shengquan Tuo <sup>||</sup>, Sokrates T. Pantelides <sup>‡||</sup>, and James H. Dickerson <sup>‡||</sup>

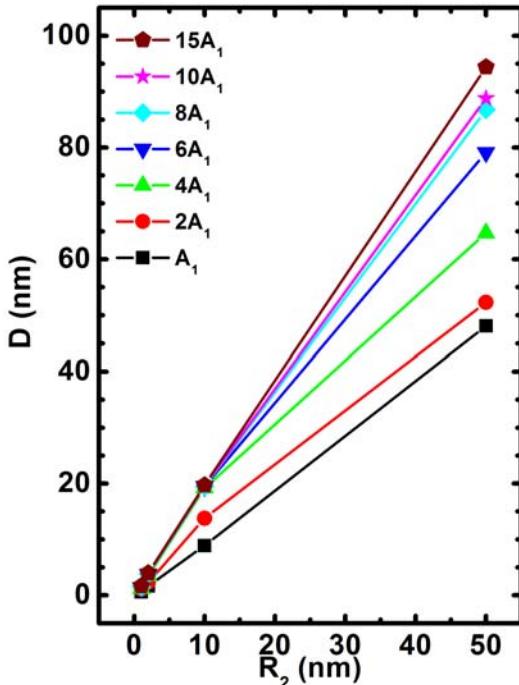
† Vanderbilt Interdisciplinary Program in Materials Science, Vanderbilt University, Nashville, Tennessee 37234-0106

‡ Vanderbilt Institute of Nanoscale Science and Engineering, Vanderbilt University, Nashville, Tennessee 37234-0106

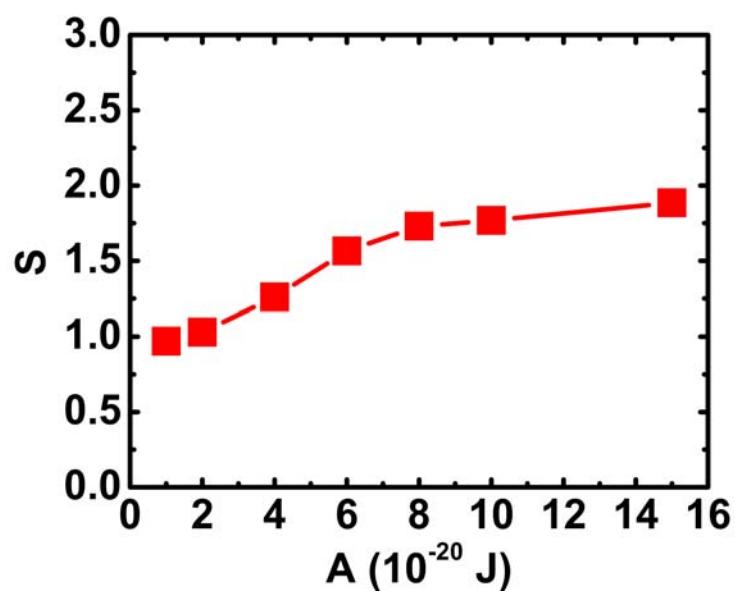
|| Department of Physics and Astronomy, Vanderbilt University, Vanderbilt University, Nashville, Tennessee 37235-1807

Eq. S1:

$$\left\{ \begin{array}{l}
 \frac{1}{R_0^3} \left( (L/2)^3 - 3C(L/2)^2 - 3R_2^2(L/2) + 3(C^2 + 4R_0^2)(L/2) - 12CR_0^2 \right) \\
 \left[ \tan^{-1} \left( \frac{R_0}{\sqrt{(L/2)^2 - 2R(L/2) - R_0^2 + R^2}} \right) - \right. \\
 \left. i \ln \left( \frac{2R_0^2 \left( \sqrt{(L/2)^2 - 2R(L/2) - R_0^2 + R^2} - iR_0 \right)}{\left( (L/2)^3 - 3C(L/2)^2 - 3R_2^2(L/2) + 3(C^2 + 4R_0^2)(L/2) - 12CR_0^2 \right) \left( R - (L/2) \right)} \right) \right] \\
 + 8 \ln \left( 2 \left( -(L/2) + R + \sqrt{(L/2)^2 - 2R(L/2) - R_0^2 + R^2} \right) \right) + \\
 - \frac{2\pi^2 q^2 \lambda}{C} \frac{1}{24} \left\{ \frac{1}{R_0^3} \left( (L/2)^3 + 3C(L/2)^2 - 3R_2^2(L/2) + 3(C^2 + 4R_0^2)(L/2) + 12CR_0^2 \right) \right. \\
 \left[ \tan^{-1} \left( \frac{R_0}{\sqrt{(L/2)^2 + 2R(L/2) - R_0^2 + R^2}} \right) - \right. \\
 \left. i \ln \left( \frac{2R_0^2 \left( \sqrt{(L/2)^2 + 2R(L/2) - R_0^2 + R^2} - iR_0 \right)}{\left( (L/2)^3 + 3C(L/2)^2 - 3R_2^2(L/2) + 3(C^2 + 4R_0^2)(L/2) + 12CR_0^2 \right) \left( R + (L/2) \right)} \right) \right] \\
 - 8 \ln \left( 2 \left( (L/2) + R + \sqrt{(L/2)^2 + 2R(L/2) - R_0^2 + R^2} \right) \right) + \\
 \left. \left[ \frac{2((L/2) - C)^2 - R_2^2}{((L/2) - R)^3} - \frac{R}{R_0^2} + \right. \right. \\
 \left. \left. \frac{5R_2^2 - 5(L/2)^2 - 5C^2 + 6R_0^2 + 10(L/2)C}{R_0^2((L/2) - R)} + \right. \right. \\
 \left. \left. \frac{3C - 2(L/2)}{R_0^2} + \frac{6(C - (L/2))}{((L/2) - R)^2} \right] \right\}_{C=R_2}^{C+R_2}
 \end{array} \right\}_{C-R_2}$$



**Fig. S1.** Plots of  $D$  vs.  $R_2$  at different  $A_s$  and fixed AR of 10.  $A_1=10^{-20}$  J. The plots give linear expressions between  $D$  and  $R_2$ :  $D = x+y R_2$ , where the slope  $S=y$ .



**Fig. S2.** Plots of  $S$  vs.  $A$  with fixed AR based on the expressions  $D = x+y R_2$ , where the slope  $S=y$ .

## Derivation of analytical expression of vdw force between a nanorod and nanosphere with a random configuration:

The general equation of vdw force between two objects is:

$$E = - \int_{V_1} dv_1 \int_{V_2} dv_2 \frac{q^2 \lambda}{r^6}$$

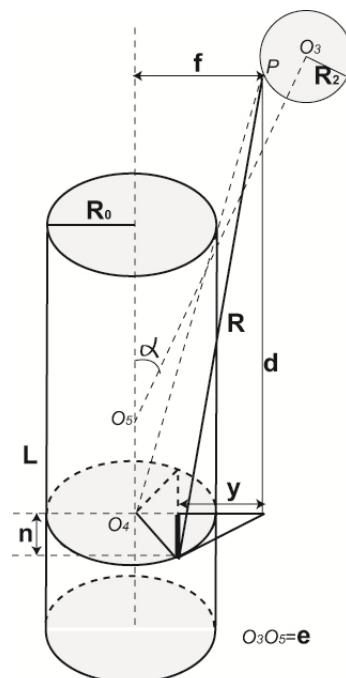
The vdw force between a nanorod and a nanosphere which is slightly off the axis of the nanorod has been derived as follows. First the total contribution of a nanorod to a point on the nanosphere can be written as:

$$E_{\text{point}} = \int_V dV \frac{q^2 \lambda}{R^6}$$

and expanded the integration in detail:

$$E_{\text{point}} = \int dl \int dy \int dn \frac{q^2 \lambda}{R^6}$$

In the above equation,  $n$  stands for the string on the circle, which is the horizontal cross-section of the cylinder, and  $y$  stands for the horizontal distance from the observed point  $P$  to the string and  $l$  stands for the height of the nanorod. The configuration shows as follows:



$$R = \sqrt{y^2 + d^2 + n^2}$$

$$n_{\max} = \sqrt{b^2 - (f - y)^2}$$

$$E_{po\text{ int}} = q^2 \lambda \int dl \int dy \cdot 2 \int_0^{\sqrt{b^2 - (f - y)^2}} dn \frac{1}{(y^2 + d^2 + n^2)^3}$$

$$\begin{aligned} \int_0^{\sqrt{b^2 - (f - y)^2}} dn \frac{1}{(d^2 + y^2 + n^2)^3} &= \frac{1}{4} \left[ \frac{3 \arctan\left(\frac{n}{\sqrt{d^2 + y^2}}\right)}{(d^2 + y^2)^{\frac{5}{2}}} + \right. \\ &\quad \left. \frac{n \cdot (5d^2 + 5y^2 + 3n^2)}{(d^2 + y^2)^2 \cdot (d^2 + y^2 + n^2)^2} \right]_0^{\sqrt{b^2 - (f - y)^2}} \\ &= \frac{1}{4} \left[ \frac{3 \arctan\left(\frac{\sqrt{b^2 - (f - y)^2}}{\sqrt{d^2 + y^2}}\right)}{(d^2 + y^2)^{\frac{5}{2}}} + \right. \\ &\quad \left. \frac{\sqrt{b^2 - (f - y)^2} \cdot (5d^2 + 5y^2 + 3 \cdot (b^2 - (f - y)^2))}{(d^2 + y^2)^2 \cdot (d^2 + y^2 + (b^2 - (f - y)^2))^2} \right] \end{aligned}$$

$R$  can be expressed in terms of  $y, d, n$ , and we get:

The maximum of the string is ( $b$  is the radius of the rod):

So the total contribution of a string on the circle is:

The factor 2 is given due to the symmetry contribution of the string. This gives us the result:

$$E_{\text{point}} = q^2 \lambda \int dl \int dx \frac{1}{4} \left( \begin{array}{l} \frac{3 \arctan(\frac{\sqrt{b^2 - (f-x)^2}}{\sqrt{d^2 + x^2}})}{(d^2 + x^2)^{\frac{5}{2}}} + \\ \frac{\sqrt{b^2 - (f-x)^2} \cdot (5d^2 + 5x^2 + 3 \cdot (b^2 - (f-x)^2))}{(d^2 + x^2)^2 \cdot (d^2 + x^2 + (b^2 - (f-x)^2))^2} \end{array} \right)$$

Subsitute it back to the integration, we get:

$$E_{\text{point}} = q^2 \lambda \int dl \int dx \frac{1}{4} \left( \begin{array}{l} \frac{3 \arctan(\frac{\sqrt{b^2 - f^2 + 2fx}}{d})}{d^5} + \\ \frac{\sqrt{b^2 - f^2 + 2fx} \cdot (5d^2 + 3 \cdot (b^2 - f^2 + 2fx))}{d^4 \cdot (d^2 + b^2 - f^2 + 2fx)^2} \end{array} \right)$$

The next step is to calculate the vdw force contribution of the circle. The y direction has been chosen to integrate to get the contribution of the the total area of the circle. The integration is: (We use mathematica to calculate the intergral, to facilitate the calculation we set  $y=x$ ,  $dy=dx$ )

$$E_{\text{point}} = q^2 \lambda \int dl \int dy \frac{1}{4} \left( \begin{array}{l} \frac{3 \arctan(\frac{\sqrt{b^2 - (f-y)^2}}{\sqrt{d^2 + y^2}})}{(d^2 + y^2)^{\frac{5}{2}}} + \\ \frac{\sqrt{b^2 - (f-y)^2} \cdot (5d^2 + 5y^2 + 3 \cdot (b^2 - (f-y)^2))}{(d^2 + y^2)^2 \cdot (d^2 + y^2 + (b^2 - (f-y)^2))^2} \end{array} \right)$$

It is very hard to integrate this equation. A reasonable assumption can be made here that the nanosphere is so close to the nanorod so that the higher order of  $x$  can be igored all:

The result is listed below:

$$\int dx \frac{1}{4} \left\{ \begin{array}{l} \frac{3 \arctan(\frac{\sqrt{b^2 - f^2 + 2fx}}{d})}{d^5} + \\ \frac{\sqrt{b^2 - f^2 + 2fx} \cdot (5d^2 + 3 \cdot (b^2 - f^2 + 2fx))}{d^4 \cdot (d^2 + b^2 - f^2 + 2fx)^2} \end{array} \right\} =$$

$$\left\{ \begin{array}{l} \frac{(b^2 - f^2 + 2fx)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{b^2 - f^2 + 2fx}{d^2}\right]}{fd} + \\ \frac{0.667 \cdot (b^2 - f^2 + 2fx)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{b^2 - f^2 + 2fx}{d^2}\right]}{fd} + \\ \frac{1}{4d^5} \left\{ \begin{array}{l} 3x \cdot \arctan(\frac{\sqrt{b^2 - f^2 + 2fx}}{d}) - \frac{3}{fd \sqrt{b^2 - f^2 + 2fx}} \cdot (-0.333b^4 + \\ (0.5f^2 - 0.5b^2)(b^2 - f^2 + 2fx) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{b^2 - f^2 + 2fx}{d^2}\right] + \\ 0.167 \cdot (b^2 - f^2 + 2fx)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{b^2 - f^2 + 2fx}{d^2}\right] + \\ 0.5b^2 \cdot (b^2 - f^2 + 2fx) - 0.167 \cdot (b^2 - f^2 + 2fx)^2 - 0.5f^2 \cdot (b^2 - f^2 + 2fx) + \\ 0.667 \cdot b^2 f^2 - 0.333b^2 fx - 0.333f^4 + 0.333f^3 x + 0.667f^2 x^2 \end{array} \right\} \end{array} \right\}$$

Then put the upper limit, which is the furthest point from the observed point  $P$  ( $x=f+b$ ) and lower limit, which is the nearest point ( $x=f-b$ ), into  $x$ , the complete integration as a function of  $d$  can be written as:

$$\begin{aligned}
 & \left\{ \frac{(b^2 - f^2 + 2f(f+b))^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{b^2 - f^2 + 2f(f+b)}{d^2}\right]}{fd} + \right. \\
 & \quad \frac{0.667 \cdot (b^2 - f^2 + 2f(f+b))^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{b^2 - f^2 + 2f(f+b)}{d^2}\right]}{fd} + \\
 & \quad \frac{1}{4d^5} \left\{ 3(f+b) \cdot \arctan\left(\frac{\sqrt{b^2 - f^2 + 2f(f+b)}}{d}\right) - \frac{3}{fd\sqrt{b^2 - f^2 + 2f(f+b)}} \cdot (-0.333b^4 + \right. \\
 & \quad (0.5f^2 - 0.5b^2)(b^2 - f^2 + 2f(f+b)) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{b^2 - f^2 + 2f(f+b)}{d^2}\right] + \\
 & \quad 0.167 \cdot (b^2 - f^2 + 2f(f+b))^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{b^2 - f^2 + 2f(f+b)}{d^2}\right] + \\
 & \quad 0.5b^2 \cdot (b^2 - f^2 + 2f(f+b)) - 0.167 \cdot (b^2 - f^2 + 2f(f+b))^2 - 0.5f^2 \cdot (b^2 - f^2 + 2f(f+b)) + \\
 & \quad \left. 0.667 \cdot b^2 f^2 - 0.333b^2 f(f+b) - 0.333f^4 + 0.333f^3(f+b) + 0.667f^2(f+b)^2 \right\} \\
 & \quad \left. \frac{(b^2 - f^2 + 2f(f-b))^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{b^2 - f^2 + 2f(f-b)}{d^2}\right]}{fd} + \right. \\
 & \quad \frac{0.667 \cdot (b^2 - f^2 + 2f(f-b))^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{b^2 - f^2 + 2f(f-b)}{d^2}\right]}{fd} + \\
 & \quad \frac{1}{4d^5} \left\{ 3(f-b) \cdot \arctan\left(\frac{\sqrt{b^2 - f^2 + 2f(f-b)}}{d}\right) - \frac{3}{fd\sqrt{b^2 - f^2 + 2f(f-b)}} \cdot (-0.333b^4 + \right. \\
 & \quad (0.5f^2 - 0.5b^2)(b^2 - f^2 + 2f(f-b)) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{b^2 - f^2 + 2f(f-b)}{d^2}\right] + \\
 & \quad 0.167 \cdot (b^2 - f^2 + 2f(f-b))^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{b^2 - f^2 + 2f(f-b)}{d^2}\right] + \\
 & \quad 0.5b^2 \cdot (b^2 - f^2 + 2f(f-b)) - 0.167 \cdot (b^2 - f^2 + 2f(f-b))^2 - 0.5f^2 \cdot (b^2 - f^2 + 2f(f-b)) + \\
 & \quad \left. 0.667 \cdot b^2 f^2 - 0.333b^2 f(f-b) - 0.333f^4 + 0.333f^3(f-b) + 0.667f^2(f-b)^2 \right\}
 \end{aligned}$$

Then put  $d$  as the variable  $x$  ( $d=x$ ) and integrate the above equation so that the total vdw force contribution of a nanorod to the observed point  $P$  can be calculated. The result is:

$$\begin{aligned}
 F(x) = & \frac{1}{4fx^5} \left\{ \frac{0.2b^4}{(b^2 + 2bf - 3f^2)^{0.5}} + \frac{0.2b^3 f}{(b^2 + 2bf - 3f^2)^{0.5}} - \frac{b^2 f^2}{(b^2 + 2bf - 3f^2)^{0.5}} + \frac{0.6bf^3}{(b^2 + 2bf - 3f^2)^{0.5}} \right. \\
 & + \frac{6.661 * 10^{-17} f^4}{(b^2 + 2bf - 3f^2)^{0.5}} - 0.3b^2(b^2 + 2bf - 3f^2)^{0.5} + 0.3f^2(b^2 + 2bf - 3f^2)^{0.5} + 0.1(b^2 + 2bf - 3f^2)^{1.5} \\
 & - \frac{0.2b^4}{(b^2 + 2bf + f^2)^{0.5}} - \frac{0.2b^3 f}{(b^2 + 2bf + f^2)^{0.5}} + \frac{0.6b^2 f^2}{(b^2 + 2bf + f^2)^{0.5}} + \frac{bf^3}{(b^2 + 2bf + f^2)^{0.5}} + \frac{0.4f^4}{(b^2 + 2bf + f^2)^{0.5}} \\
 & + 0.3b^2(b^2 + 2bf + f^2)^{0.5} - 0.3f^2(b^2 + 2bf + f^2)^{0.5} - 0.1(b^2 + 2bf + f^2)^{1.5} \\
 & + 0.332(b^2 + 2bf - 3f^2)^{1.5} \text{HypergeometricPFQ Regularized} \left[ \{1.5, 1\}, \{3.5\}, -\frac{b^2 + 2bf - 3f^2}{x^2} \right] \\
 & - 0.332(b^2 + 2bf + f^2)^{1.5} \text{HypergeometricPFQ Regularized} \left[ \{1.5, 1\}, \{3.5\}, -\frac{b^2 + 2bf + f^2}{x^2} \right] \\
 & + 0.443(b^2 + 2bf - 3f^2)^{1.5} \text{HypergeometricPFQ Regularized} \left[ \{1.5, 2\}, \{3.5\}, -\frac{b^2 + 2bf - 3f^2}{x^2} \right] \\
 & - 0.443(b^2 + 2bf + f^2)^{1.5} \text{HypergeometricPFQ Regularized} \left[ \{1.5, 2\}, \{3.5\}, -\frac{b^2 + 2bf + f^2}{x^2} \right] \\
 & + 0.884b^2(b^2 + 2bf - 3f^2)^{0.5} \text{HypergeometricPFQ Regularized} \left[ \{0.5, 1, 2.5\}, \{1.5, 3.5\}, -\frac{b^2 + 2bf - 3f^2}{x^2} \right] \\
 & - 0.884f^2(b^2 + 2bf - 3f^2)^{0.5} \text{HypergeometricPFQ Regularized} \left[ \{0.5, 1, 2.5\}, \{1.5, 3.5\}, -\frac{b^2 + 2bf - 3f^2}{x^2} \right] \\
 & - 0.884b^2(b^2 + 2bf + f^2)^{0.5} \text{HypergeometricPFQ Regularized} \left[ \{0.5, 1, 2.5\}, \{1.5, 3.5\}, -\frac{b^2 + 2bf + f^2}{x^2} \right] \\
 & + 0.884f^2(b^2 + 2bf + f^2)^{0.5} \text{HypergeometricPFQ Regularized} \left[ \{0.5, 1, 2.5\}, \{1.5, 3.5\}, -\frac{b^2 + 2bf + f^2}{x^2} \right] \}
 \end{aligned}$$

In order to simplify the result, we assume that  $f$  is very small which means the nanosphere is just slightly off the axis of the nanorod so that the aspect ratio can be defined as  $s=b/d$ , which is a constant in this step. Integrate again, the equation above can be simplified into:

$$F(x) = -\frac{1}{40fx^5} \left\{ \begin{aligned} & (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right] + \\ & 0.667 \cdot (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1} \left[ 1.5, 2, 2.5, -\frac{1}{s^2} \right] - \\ & (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right] - \\ & 0.667 \cdot (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1} \left[ 1.5, 2, 2.5, -\frac{1}{s^2} \right] + \\ & \frac{1}{\sqrt{b^2 - 3f^2 + 2bf}} \cdot (-b^4 - b^3f + -0.333f^4 + \\ & (1.5f^2 - 1.5b^2)(b^2 - 3f^2 + 2bf) \text{Hypergeometric2F1} \left[ 0.5, 1, 1.5, -\frac{1}{s^2} \right] + \\ & 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right] + \\ & 5 \cdot b^2f^2 + 1.5b^2 \cdot (b^2 - 3f^2 + 2bf) - 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 - \\ & 1.5f^2 \cdot (b^2 - 3f^2 + 2bf) - 3bf^3 - 3.33 \times 10^{-16}f^4) + \\ & \frac{1}{\sqrt{b^2 + f^2 + 2bf}} \cdot (b^4 + b^3f + \\ & (1.5b^2 - 1.5f^2)(b^2 + f^2 + 2bf) \text{Hypergeometric2F1} \left[ 0.5, 1, 1.5, -\frac{1}{s^2} \right] - \\ & 0.5 \cdot (b^2 + f^2 + 2bf)^2 \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right] - \\ & 3 \cdot b^2f^2 - 1.5b^2 \cdot (b^2 + f^2 + 2bf) + 0.5 \cdot (b^2 + f^2 + 2bf)^2 - \\ & 1.5f^2 \cdot (b^2 + f^2 + 2bf) - 5bf^3 - 2f^4) \end{aligned} \right\}$$

So the  $vdW$  force between a rod and an observed point from a nanosphere is (substitute the  $x$  with the upper limit  $t+L/2$  and lower limit  $t-L/2$  of  $x$ , where  $t$  is the separation between point  $P$  and the middle plane of the rod):

$$\begin{aligned}
 & \left\{ (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] + \right. \\
 & 0.667 \cdot (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] - \\
 & (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] - \\
 & 0.667 \cdot (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] + \\
 & \frac{1}{\sqrt{b^2 - 3f^2 + 2bf}} \cdot (-b^4 - b^3f + -0.333f^4 - 1.5f^2 \cdot (b^2 - 3f^2 + 2bf) - 3bf^3 + \\
 & \left. - \frac{1}{40f(t + \frac{L}{2})^5} \left\{ (1.5f^2 - 1.5b^2)(b^2 - 3f^2 + 2bf) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] + \right. \right. \\
 & 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] + \\
 & 5 \cdot b^2f^2 + 1.5b^2 \cdot (b^2 - 3f^2 + 2bf) - 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 - 3.33 \times 10^{-16}f^4 + \\
 & \frac{1}{\sqrt{b^2 + f^2 + 2bf}} \cdot (b^4 + b^3f - 1.5f^2 \cdot (b^2 + f^2 + 2bf) - 5bf^3 - 2f^4 + \\
 & (1.5b^2 - 1.5f^2)(b^2 + f^2 + 2bf) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] - \\
 & 0.5 \cdot (b^2 + f^2 + 2bf)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] - \\
 & \left. \left. 3 \cdot b^2f^2 - 1.5b^2 \cdot (b^2 + f^2 + 2bf) + 0.5 \cdot (b^2 + f^2 + 2bf)^2 \right\} \right. \\
 & \left. (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] + \right. \\
 & 0.667 \cdot (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] - \\
 & (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] - \\
 & 0.667 \cdot (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] + \\
 & \frac{1}{\sqrt{b^2 - 3f^2 + 2bf}} \cdot (-b^4 - b^3f + -0.333f^4 - 1.5f^2 \cdot (b^2 - 3f^2 + 2bf) - 3bf^3 + \\
 & \left. \left. - \frac{1}{40f(t - \frac{L}{2})^5} \left\{ (1.5f^2 - 1.5b^2)(b^2 - 3f^2 + 2bf) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] + \right. \right. \\
 & 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] + \\
 & 5 \cdot b^2f^2 + 1.5b^2 \cdot (b^2 - 3f^2 + 2bf) - 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 - 3.33 \times 10^{-16}f^4 + \\
 & \frac{1}{\sqrt{b^2 + f^2 + 2bf}} \cdot (b^4 + b^3f - 1.5f^2 \cdot (b^2 + f^2 + 2bf) - 5bf^3 - 2f^4 + \\
 & (1.5b^2 - 1.5f^2)(b^2 + f^2 + 2bf) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] - \\
 & 0.5 \cdot (b^2 + f^2 + 2bf)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] - \\
 & \left. \left. 3 \cdot b^2f^2 - 1.5b^2 \cdot (b^2 + f^2 + 2bf) + 0.5 \cdot (b^2 + f^2 + 2bf)^2 \right\} \right. \right.
 \end{aligned}$$

Then integrate the above equation for  $t$  is a variable( $t=x$ ):

$$\int \left( \frac{1}{40f(x+\frac{L}{2})^5} (R_2^2 - e^2 + 2ex - x^2) \right) \left( \begin{array}{l} (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] + \\ 0.667 \cdot (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] - \\ (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] - \\ 0.667 \cdot (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] + \\ \frac{1}{\sqrt{b^2 - 3f^2 + 2bf}} \cdot (-b^4 - b^3f - 0.333f^4 - 1.5f^2 \cdot (b^2 - 3f^2 + 2bf) - 3bf^3 + \\ (1.5f^2 - 1.5b^2)(b^2 - 3f^2 + 2bf) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] + \\ 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] + \\ 5 \cdot b^2f^2 + 1.5b^2 \cdot (b^2 - 3f^2 + 2bf) - 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 - 3.33 \times 10^{-16}f^4) + \\ \frac{1}{\sqrt{b^2 + f^2 + 2bf}} \cdot (b^4 + b^3f - 1.5f^2 \cdot (b^2 + f^2 + 2bf) - 5bf^3 - 2f^4 + \\ (1.5b^2 - 1.5f^2)(b^2 + f^2 + 2bf) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] - \\ 0.5 \cdot (b^2 + f^2 + 2bf)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] - \\ 3 \cdot b^2f^2 - 1.5b^2 \cdot (b^2 + f^2 + 2bf) + 0.5 \cdot (b^2 + f^2 + 2bf)^2) \end{array} \right) dx$$

$$\left. \frac{1}{40f(x-\frac{L}{2})^5} (R_2^2 - e^2 + 2ex - x^2) \right) \left( \begin{array}{l} (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] + \\ 0.667 \cdot (b^2 + f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] - \\ (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] - \\ 0.667 \cdot (b^2 - 3f^2 + 2bf)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] + \\ \frac{1}{\sqrt{b^2 - 3f^2 + 2bf}} \cdot (-b^4 - b^3f + -0.333f^4 - 1.5f^2 \cdot (b^2 - 3f^2 + 2bf) - 3bf^3 + \\ (1.5f^2 - 1.5b^2)(b^2 - 3f^2 + 2bf) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] + \\ 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] + \\ 5 \cdot b^2f^2 + 1.5b^2 \cdot (b^2 - 3f^2 + 2bf) - 0.5 \cdot (b^2 - 3f^2 + 2bf)^2 - 3.33 \times 10^{-16}f^4) + \\ \frac{1}{\sqrt{b^2 + f^2 + 2bf}} \cdot (b^4 + b^3f - 1.5f^2 \cdot (b^2 + f^2 + 2bf) - 5bf^3 - 2f^4 + \\ (1.5b^2 - 1.5f^2)(b^2 + f^2 + 2bf) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] - \\ 0.5 \cdot (b^2 + f^2 + 2bf)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] - \\ 3 \cdot b^2f^2 - 1.5b^2 \cdot (b^2 + f^2 + 2bf) + 0.5 \cdot (b^2 + f^2 + 2bf)^2) \end{array} \right)$$

The result is as follows, where  $e$  is the center-center distance between the rod and the sphere:

:

$$\begin{aligned}
 F(x) = & \frac{1}{60f(L^2 - 4x^2)^4} (-L^6 + 192x^4(r^2 - 2x^2) + 4L^4(3r^2 + 4x^2) + 48L^2(6r^2x^2 - 7x^4) \\
 & - 12e^2(L^4 + 24L^2x^2 + 16x^4) + 128e(5L^2x^3 + 4x^5)) \\
 & \left\{ -(b^2 + 2bf - 3f^2)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] \right. \\
 & +(b^2 + 2bf + f^2)^{1.5} \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] \\
 & + \frac{1}{(b^2 + 2bf - 3f^2)^{0.5}} (-b^4 - b^3f + 5b^2f^2 - 3bf^3 - 3.33 * 10^{-16}f^4 + 1.5b^2(b^2 + 2bf - 3f^2) \\
 & - 1.5f^2(b^2 + 2bf - 3f^2) - 0.5(b^2 + 2bf - 3f^2)^2 \\
 & +(b^2 + 2bf - 3f^2)(-1.5b^2 + 1.5f^2) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] \\
 & + 0.5(b^2 + 2bf - 3f^2)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] ) \\
 & + \frac{1}{(b^2 + 2bf + f^2)^{0.5}} (b^4 + b^3f - 3b^2f^2 - 5bf^3 - 2f^4 - 1.5b^2(b^2 + 2bf + f^2) \\
 & + 1.5f^2(b^2 + 2bf + f^2) + 0.5(b^2 + 2bf + f^2)^2 \\
 & +(1.5b^2 - 1.5f^2)(b^2 + 2bf + f^2) \text{Hypergeometric2F1}\left[0.5, 1, 1.5, -\frac{1}{s^2}\right] \\
 & - 0.5(b^2 + 2bf + f^2)^2 \text{Hypergeometric2F1}\left[1.5, 1, 2.5, -\frac{1}{s^2}\right] ) \\
 & - 0.667(b^2 + 2bf - 3f^2)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] \\
 & \left. + 0.667(b^2 + 2bf + f^2)^{1.5} \text{Hypergeometric2F1}\left[1.5, 2, 2.5, -\frac{1}{s^2}\right] \right\}
 \end{aligned}$$

Then the vdW force between the nanorode and the nanosphere is equal to

$$vdW = F(e + R_2) - F(e - R_2)$$

$$vdw = \left\{ \begin{array}{l} \frac{1}{60f(L^2 - 4(e + R_2)^2)^4} \left[ \begin{array}{l} (-L^6 + 192(e + R_2)^4(R_2^2 - 2(e + R_2)^2) + 4L^4(3R_2^2 + 4(e + R_2)^2) + \\ 48L^2(6R_2^2(e + R_2)^2 - 7(e + R_2)^4) - 12e^2(L^4 + 24L^2(e + R_2)^2 + \\ 16(e + R_2)^4) + 128e(5L^2(e + R_2)^3 + 4(e + R_2)^5)) \\ \{- (b^2 + 2bf - 3f^2)^{15} \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right] \\ + (b^2 + 2bf + f^2)^{15} \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right] \\ + \frac{1}{(b^2 + 2bf - 3f^2)^{0.5}} (-b^4 - b^3f + 5b^2f^2 - 3bf^3 - 3.33 * 10^{-16}f^4 + \\ 1.5b^2(b^2 + 2bf - 3f^2) \\ - 1.5f^2(b^2 + 2bf - 3f^2) - 0.5(b^2 + 2bf - 3f^2)^2 \\ + (b^2 + 2bf - 3f^2)(-1.5b^2 + 1.5f^2) \text{Hypergeometric2F1} \left[ 0.5, 1, 1.5, -\frac{1}{s^2} \right] \\ + 0.5(b^2 + 2bf - 3f^2)^2 \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right]) \\ + \frac{1}{(b^2 + 2bf + f^2)^{0.5}} (b^4 + b^3f - 3b^2f^2 - 5bf^3 - 2f^4 - 1.5b^2(b^2 + 2bf + f^2) \\ + 1.5f^2(b^2 + 2bf + f^2) + 0.5(b^2 + 2bf + f^2)^2 \\ + (1.5b^2 - 1.5f^2)(b^2 + 2bf + f^2) \text{Hypergeometric2F1} \left[ 0.5, 1, 1.5, -\frac{1}{s^2} \right] \\ - 0.5(b^2 + 2bf + f^2)^2 \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right]) \\ - 0.667(b^2 + 2bf - 3f^2)^{15} \text{Hypergeometric2F1} \left[ 1.5, 2, 2.5, -\frac{1}{s^2} \right] \\ + 0.667(b^2 + 2bf + f^2)^{15} \text{Hypergeometric2F1} \left[ 1.5, 2, 2.5, -\frac{1}{s^2} \right] \} \\ (-L^6 + 192(e - R_2)^4(R_2^2 - 2(e - R_2)^2) + 4L^4(3R_2^2 + 4(e - R_2)^2) + \\ 48L^2(6R_2^2(e - R_2)^2 - 7(e - R_2)^4) - 12e^2(L^4 + 24L^2(e - R_2)^2 + \\ 16(e - R_2)^4) + 128e(5L^2(e - R_2)^3 + 4(e - R_2)^5)) \\ \{- (b^2 + 2bf - 3f^2)^{15} \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right] \\ + (b^2 + 2bf + f^2)^{15} \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right] \\ + \frac{1}{(b^2 + 2bf - 3f^2)^{0.5}} (-b^4 - b^3f + 5b^2f^2 - 3bf^3 - 3.33 * 10^{-16}f^4 + \\ 1.5b^2(b^2 + 2bf - 3f^2) \\ - 1.5f^2(b^2 + 2bf - 3f^2) - 0.5(b^2 + 2bf - 3f^2)^2 \\ + (b^2 + 2bf - 3f^2)(-1.5b^2 + 1.5f^2) \text{Hypergeometric2F1} \left[ 0.5, 1, 1.5, -\frac{1}{s^2} \right] \\ + 0.5(b^2 + 2bf - 3f^2)^2 \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right]) \\ + \frac{1}{(b^2 + 2bf + f^2)^{0.5}} (b^4 + b^3f - 3b^2f^2 - 5bf^3 - 2f^4 - 1.5b^2(b^2 + 2bf + f^2) \\ + 1.5f^2(b^2 + 2bf + f^2) + 0.5(b^2 + 2bf + f^2)^2 \\ + (1.5b^2 - 1.5f^2)(b^2 + 2bf + f^2) \text{Hypergeometric2F1} \left[ 0.5, 1, 1.5, -\frac{1}{s^2} \right] \\ - 0.5(b^2 + 2bf + f^2)^2 \text{Hypergeometric2F1} \left[ 1.5, 1, 2.5, -\frac{1}{s^2} \right]) \\ - 0.667(b^2 + 2bf - 3f^2)^{15} \text{Hypergeometric2F1} \left[ 1.5, 2, 2.5, -\frac{1}{s^2} \right] \\ + 0.667(b^2 + 2bf + f^2)^{15} \text{Hypergeometric2F1} \left[ 1.5, 2, 2.5, -\frac{1}{s^2} \right] \} \end{array} \right] \end{array} \right\}$$