

# Manual for vdWnano software

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## 1 Introduction

This document provides instructions for the installation and usage of vdWnano MATLAB application. This application computes the van der Waals (vdW) interaction energies between nanocubes by implementing the analytical model described in Lee and Arya<sup>1</sup>. The application has been developed using MATLAB App Designer and has been packaged as MATLAB application files. Two versions of the software exist. The first version vdWnano has the complete graphical user interface (GUI) and is recommended for users with MATLAB 2019a or later versions. The vdWnano\_simple is a simpler version without several components of the GUI. This version is recommended for users with older versions of MATLAB. The backward compatibility of vdWnano\_simple has been verified for MATLAB 2017b.

The application is open-source and available at:

<https://github.com/BrianHLeeProjects/vdWnano>.



Figure 1: Icon for installing the application in MATLAB.

## 2 Installation

For installation of the software, open MATLAB and choose the APPS tab from the MATLAB Toolstrip (Fig. 1). Click on the Install App icon and choose the vdWnano.mlappinstall or vdWnano\_simple.mlappinstall file. The application will become available for usage in the APPS tab.

## 3 Graphical User Interface

The GUI of the vdWnano application is depicted in Fig. 2. The numerical labels in the figure correspond to:

- 1 Current status of the application. The default status is Idle. Computing atomistic summation: X% completed is displayed when Compute atomistic button (6) is pressed and the energy is being calculated atomistically. Computing parameters is displayed when Enter parameters button (7) is pressed with the Recalibrate option (7a).

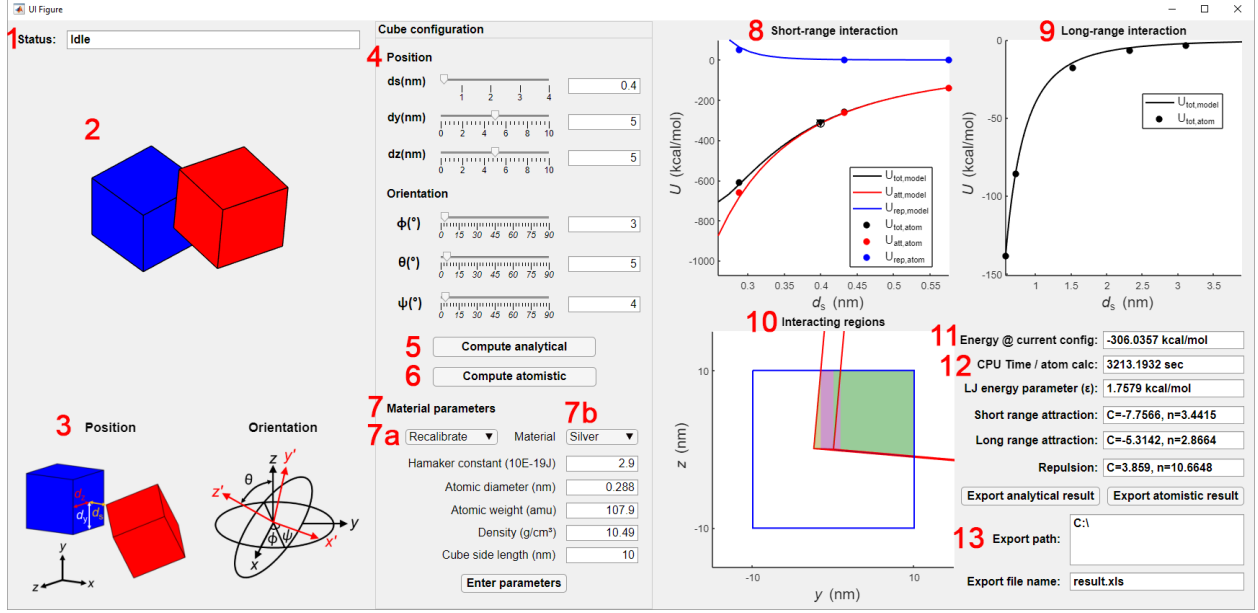


Figure 2: Graphical user interface of the MATLAB application.

- 2 Depiction of the cubes with the configuration specified in 4. The perspective can be rotated by clicking and dragging the figure with the mouse.
- 3 Diagram explaining the coordinate system used in the application. The center of mass of the blue cube is at the origin and its facets are parallel to the  $x$ ,  $y$ ,  $z$  axes. The position of the red cube is described by the position of its vertex that is closest to the interacting facet of the blue cube. The variables  $d_s$ ,  $d_y$ , and  $d_z$  are used to describe this vertex position. The orientation of the red cube is described by the Euler angles  $\phi$ ,  $\theta$ , and  $\psi$  using the  $x$ -convention.
- 4 The position ( $d_s$ ,  $d_y$ ,  $d_z$ ) and orientation ( $\phi$ ,  $\theta$ ,  $\psi$ ) of the red cube can be specified using either the slides or the text boxes in this region. The selected configuration is depicted in 2 when the values are changed either through the slides or the text boxes.
- 5 The energies for the configuration ( $d_y$ ,  $d_z$ ,  $\phi$ ,  $\theta$ ,  $\psi$ ) from 4 and  $d_s$  varying from  $0.7\sigma$  to  $0.4D$  are computed using the analytical model and plotted on 8 and 9 as solid lines. Here,  $\sigma$  and  $D$  represent the diameter of the atoms and the side length of the cube, respectively. These values can be specified in 7. The energy at the  $d_s$  specified in 4 is also computed and plotted as an unfilled circle on 8 or 9. The numerical value of this energy is displayed on 11.
- 6 The energies for the configuration ( $d_y$ ,  $d_z$ ,  $\phi$ ,  $\theta$ ,  $\psi$ ) specified in 4 and  $d_s$  varying from  $0.7\sigma$  to  $0.4D$  are computed as the sum of Lennard Jones (LJ) potentials of atoms and plotted on 8 and 9 as scatter points. The energy at the  $d_s$  specified in 4 is also computed and plotted as a downward-pointing triangle on 8 or 9. The numerical value of this energy is displayed on 11. The computational cost for this process is  $O(D^6)$  and it is recommended that this function is used only when the cube length is less than  $30\sigma$ .
- 7 Material parameters including the Hamaker constant, atomic diameter ( $\sigma$ ), atomic weight, mass density of the material, and the side length of the cubes ( $D$ ) can be specified. The parameters for silver, gold, copper, and silica can be loaded from the material option (7b). The drop-down option of 7a allows the user to choose either the default values or recalibrated values of the  $C$  and  $n$  parameters for  $U_{rod}$ .

These parameters are the internal variables used to fit the cube-rod interaction energy with a power-law model. The default values correspond to the  $C$  and  $n$  obtained from cube-rod interactions with cube lengths equal to  $50\sigma$ . Enter parameters button must be pressed for the parameters to be updated.

- 8 The short-range ( $0.7\sigma < d_s < 2.0\sigma$ ) interaction energies for the configurations from 4 are plotted. Red, blue, and black plots represent the attractive energies ( $U_{\text{att}}$ ), the repulsive energies ( $U_{\text{rep}}$ ), and the total energies ( $U_{\text{tot}}$ ), respectively.
- 9 The long-range ( $2.0\sigma < d_s < 0.4D$ ) interaction energies for the configurations from 4 are plotted. Only  $U_{\text{tot}}$  is plotted as  $U_{\text{rep}}$  is negligible and  $U_{\text{att}} \approx U_{\text{tot}}$ .
- 10 The  $y$ - $z$  projection of the interacting faces are plotted. The shaded areas represent the regions in which the integrands and the limits of the integrals for the analytical model are equivalent.
- 11 The energy for the configuration ( $d_s, d_y, d_z, \phi, \theta, \psi$ ) specified in 4 is displayed. The displayed energy is from the most recent calculation. If 5 is pressed recently, the energy is obtained through the analytical model. If the most recent calculation was from 6, the energy from atomistic calculation is shown. The energy is also marked in the graph of either 8 or 9 as a black unfilled circle for analytical model and downward-pointing triangle for the atomistic calculation.
- 12 The estimated computational time for atomistic calculations,  $\varepsilon$  for the specified material parameters,  $C$  and  $n$  parameters for the  $U_{\text{rod}}$  are displayed. The values are updated when Enter parameters button from 7 is pressed.
- 13 The energy obtained from either the analytical model or the atomistic calculation is exported. The folder and the file name for the exported file is specified in the text boxes. The first three columns of the exported data represent  $d_s, d_y, d_z$  in units of nanometers (nm). Next three columns represent  $\phi, \theta, \psi$  in units of degrees ( $^\circ$ ). Last three columns correspond to  $U_{\text{att}}, U_{\text{rep}}, U_{\text{tot}}$  in units of kcal/mol. The last row correspond to the data for the configuration specified in 4. Files with the following extensions are supported: .txt, .dat, .csv, .xls, .xlsm, .xlsx, and .xlsb.

The vdWnano\_simple lacks the GUI components of 2 and 3. Otherwise, the two versions of the software are equivalent.

## References

- <sup>1</sup> Lee, B. H.; Arya G. *Analytical van der Waals interaction potential for faceted nanoparticles*. Submitted.