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[1]. 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**).

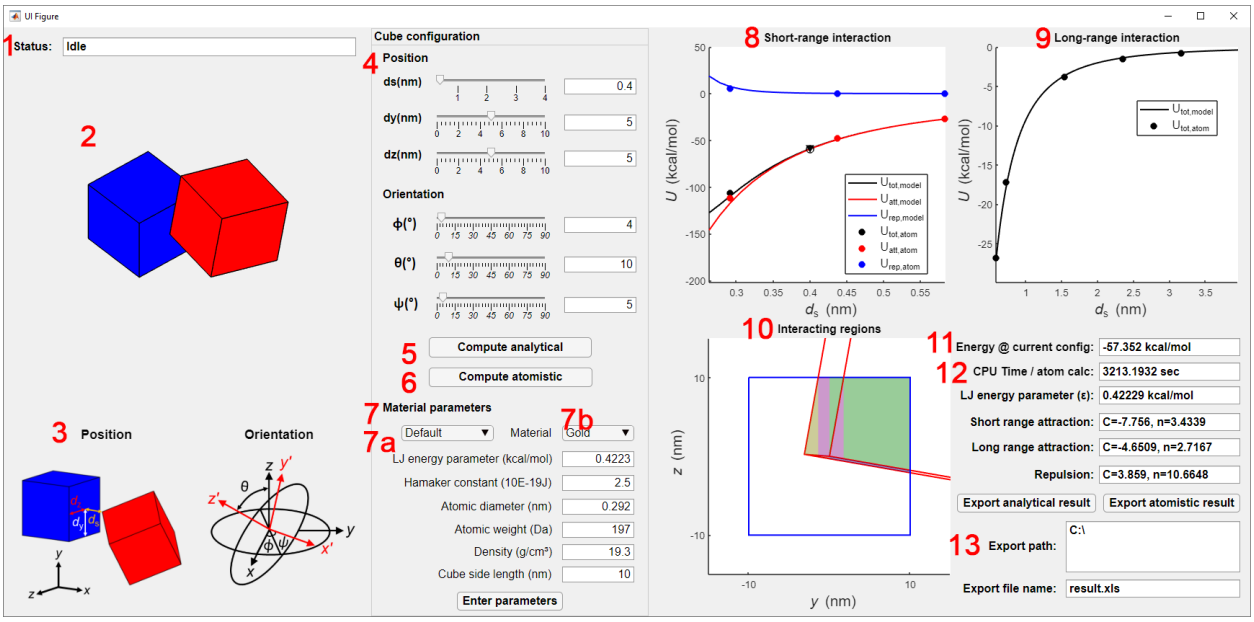

Figure 2: Graphical user interface of the MATLAB application.

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 ϕ, θ, and ψ using the x-convention.

4 The position (d_s, d_y, d_z) and orientation (ϕ, θ, ψ) 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, ϕ, θ, ψ) from **4** and d_s varying from 0.7σ to $0.4D$ are computed using the analytical model and plotted on **8** and **9** as solid lines. Here, σ 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, ϕ, θ, ψ) specified in **4** and d_s varying from 0.7σ 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 30σ.

7 LJ parameters (ε and σ) along with the cube side length (D) can be specified. If the LJ energy parameter box is filled with non-zero value, the specified ε is used by the application. If the inputted value of ε is equal to 0, the application derives ε from other material parameters including the Hamaker constant, atomic diameter (σ), atomic weight, and mass density of the material. 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 50σ. Enter parameters button must be pressed for the parameters to be updated.

8 The short-range ($0.7\sigma < d_{\mathrm{s}} < 2.0\sigma$) interaction energies for the configurations from **4** are plotted. Red, blue, and black plots represent the attractive energies (U_{att}), the repulsive energies (U_{rep}), and the total energies (U_{tot}), respectively.

9 The long-range ($2.0\sigma < d_{\mathrm{s}} < 0.4D$) interaction energies for the configurations from **4** are plotted. Only U_{tot} is plotted as U_{rep} is negligible and $U_{\mathrm{att}} \approx U_{\mathrm{tot}}$.

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}, ϕ, θ, ψ) 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, ε for the specified material parameters, C and n parameters for the U_{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 ϕ, θ, ψ in units of degrees (°). Last three columns correspond to U_{att}, U_{rep}, U_{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

[1] Lee, B. H.; Arya G. *Analytical van der Waals interaction potential for faceted nanoparticles.* Submitted.