NanoConstruct: A toolbox for the digital reconstruction of Energy Minimized NanoParticles, Nanosheets and NanoTubes Powered by Enalos Cloud Platform

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Description of NanoConstruct tools powered by Enalos Cloud Platform

Computational tools have been widely used for predicting material properties in the past. Nowadays, the rapid development of computers has increased interest in these tools due to their speed and low cost compared to physical experiments. Furthermore, mixing nanomaterials with other materials to create sols, emulsions, gels, or foams can lead to improved material properties. Efficient computational screening techniques are needed to quickly discover the most promising combinations. Atomistic simulations can be used for the screening process after digitally reconstructing the systems to be investigated. However, digitally reconstructing systems containing secondary phases, such as Nanoparticles (NPs), Nanosheets (NSs), and/or Nanotubes (NTs), is not a straightforward task. NanoConstruct, a toolbox powered by the Enalos Cloud Platform (enaloscloud.novamechanics.com), has been developed to overcome this barrier. NanoConstruct uses Crystallographic Information Files available on crystallographic databases as input to geometrically reconstruct crystalline NPs, while maintaining stoichiometry by removing excess atoms on the surface. Additionally, NanoConstruct searches the OPENKIM database and selects the Force-Field (FF) that is less generic and simultaneously contains every chemical element of the NP. The option to select a different OPENKIM FF than the suggested one is also available. After the FF selection, energy minimization is applied to investigate the NP's stability, while several descriptors are calculated for subsequent Machine Learning analysis. A similar procedure is applied for the NS and NT construction.

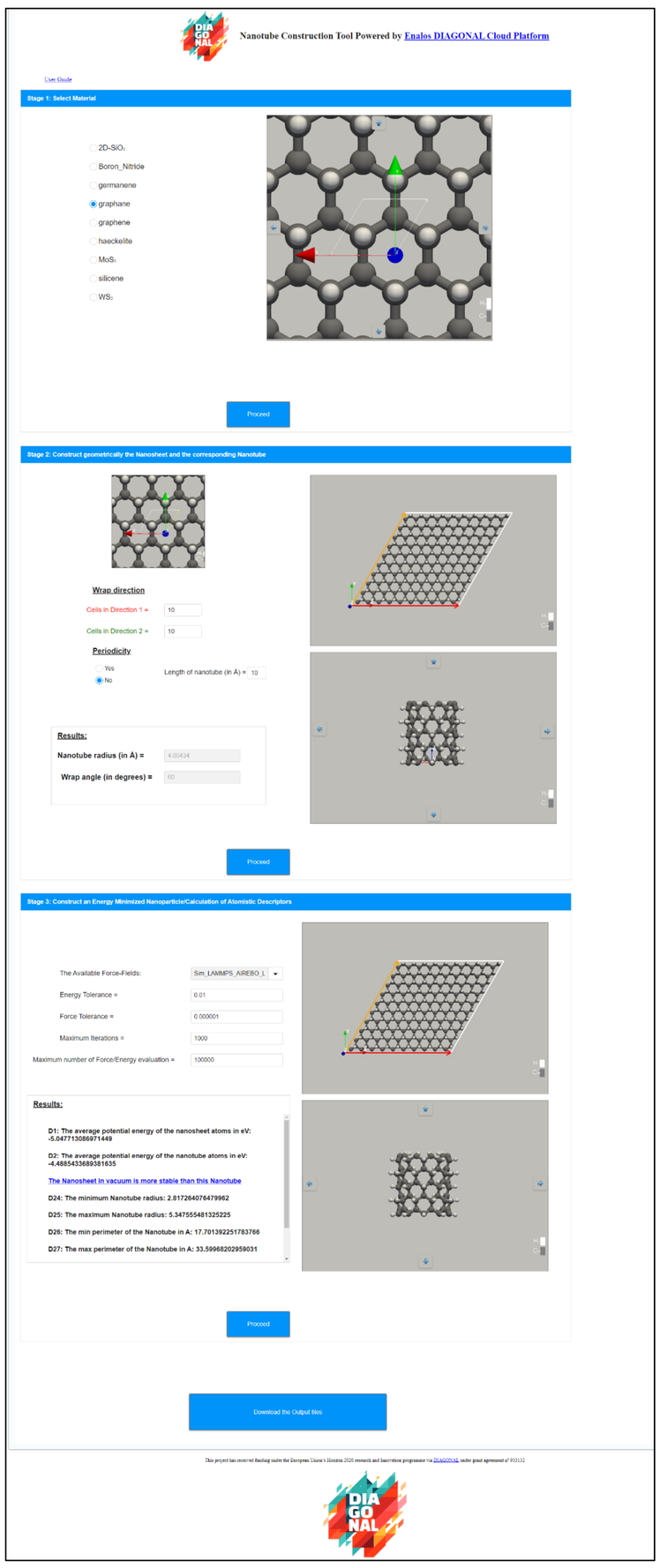

Figure 1. *Graphical user interface (GUI) of the NanoTube construction tool for the digital reconstruction of nanosheets and nanotubes which is available through the* **Enalos Cloud Platform***. The user selects among nine 2-dimensional materials (i.e. 2D-silica, haeckelite, graphene, graphene, boron nitride, germanene, silicene, molybnene disulfide and tungsten disulfide) and appears the unit cell at the top of the page. Next the user selects the wrapping direction of the unit cell by typing the unit cell replication per direction x and y. In addition, the user defines the length of the nanotube that will be reconstructed or selects to make the unit cell of the nanotube. The result of the reconstruction appears, and the user can rotate the reconstructed structures. Next, the user selects an available Force-Field to apply energy minimization into the nanotube and the nanosheet to get energy minimized structures and their atomistic descriptors which are available for download.*

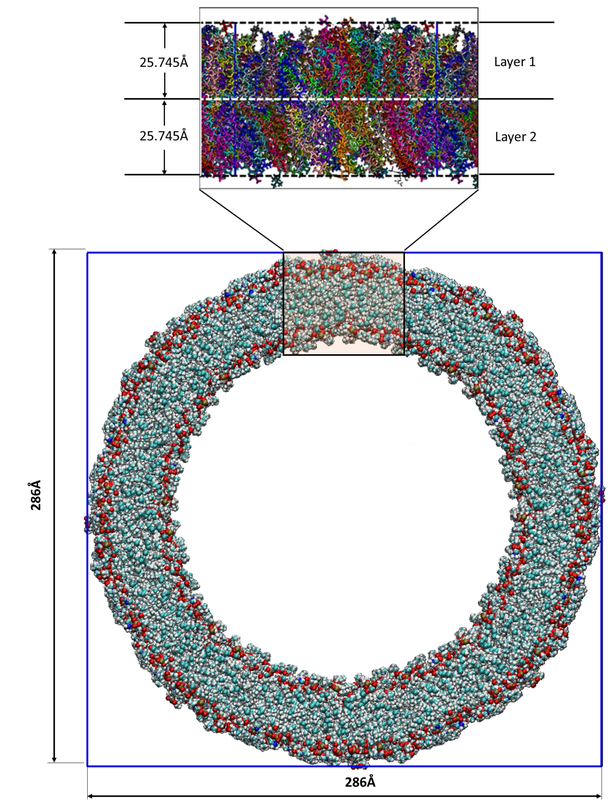

Figure 2. *Nanotube construction of 1,2-Dioleoyl-sn-glycero-3-phosphocholine (DOPC) membrane by applying the procedure of Figure 1 using the application programming Interface (API) of the Nanotube Construction tool. The bilayer of the DOPC membrane unit cell which is illustrated at the top was inserted as input. The digital reconstructed DOPC resembles the curvature of real cell membranes, and it can be used for molecular dynamics simulations.*

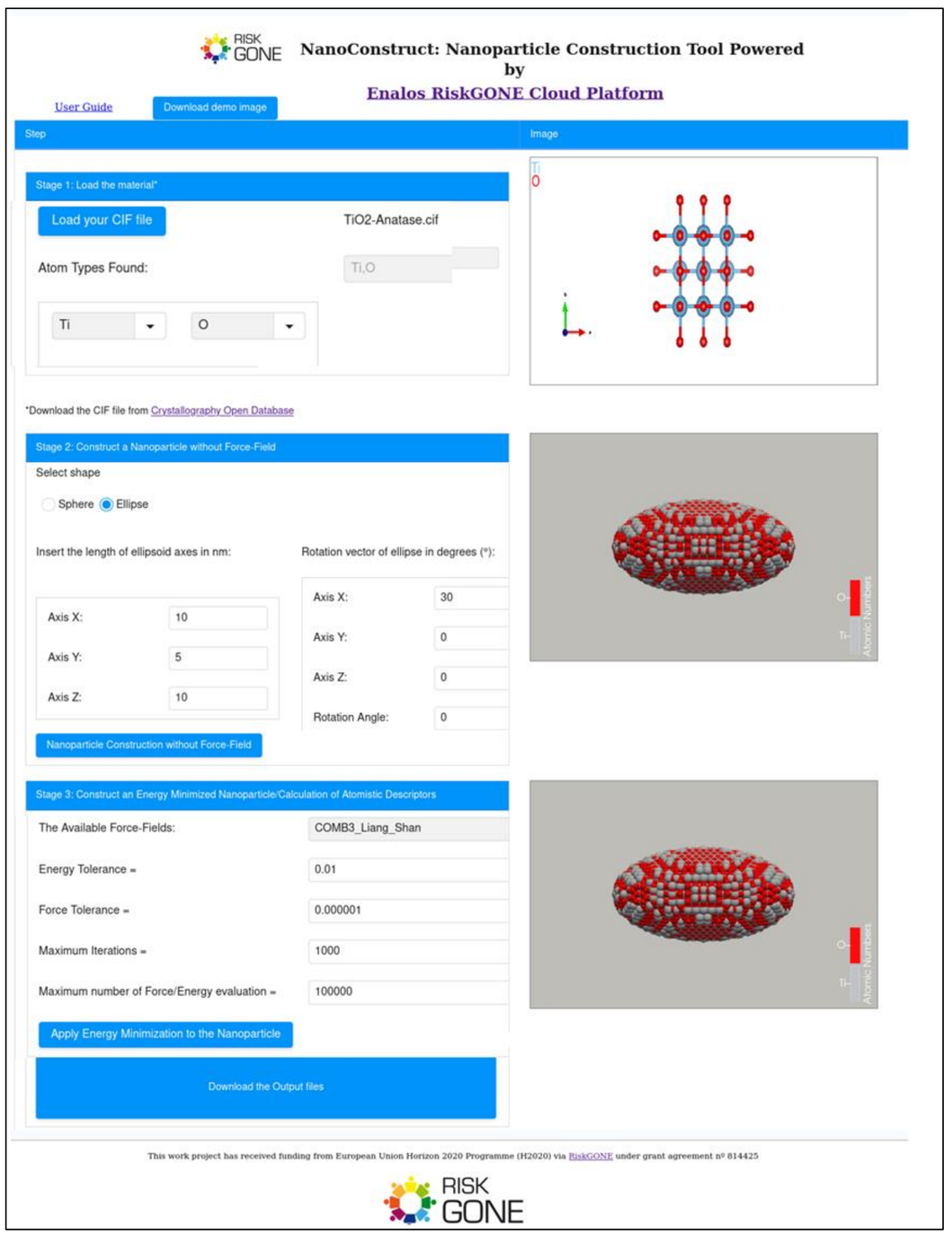

Figure 3. *Graphical user interface (GUI) of the NanoConstruct: Nanoparticle construction tool for the digital reconstruction of ellipsoidal nanoparticles which is available through the* **Enalos Cloud Platform***. The user initially loads the CIF file of the material which can be downloaded from the crystallography open database. Next, the chemical elements of the material appear which can be replaced by other elements of the same group of the periodic table. This option helps to the investigation of materials which could be stable but may not be synthesized yet. Next, an ellipsoid nanoparticle is reconstructed geometrically after the user inserts the ellipsoid lengths and the ellipsoid rotation axis. Next, the available force-fields for this material appear and the user selects one to digitally reconstruct energy minimized ellipsoid nanoparticles and to calculate their atomistic descriptors which are available for download.*

Enalos Cloud Platform, developed by NovaMechanics Ltd, is an advanced cheminformatics and nanoinformatics cloud platform available online and free of charge. It hosts a broad range of predictive models, which are provided as web services, and offers flexible and powerful cloud computing resources that reduce the barriers to entry for complex scientific calculations. Enalos Cloud Platform provides scientists with the ability to reference disparate sources of data, which can greatly aid in computer-aided drug discovery, materials design, and patient stratification decision-making processes. The platform offers a user-friendly environment that is specifically designed for non-informatics experts and provides access to state-of-the-art modeling tools for hazard prediction and risk assessment. Through Enalos Cloud Platform, any model can be made available under the technology of Software as a Service (SaaS), allowing for greater accessibility and ease of use for researchers and scientists alike.

Access the Enalos cloud Platform using this QR code

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