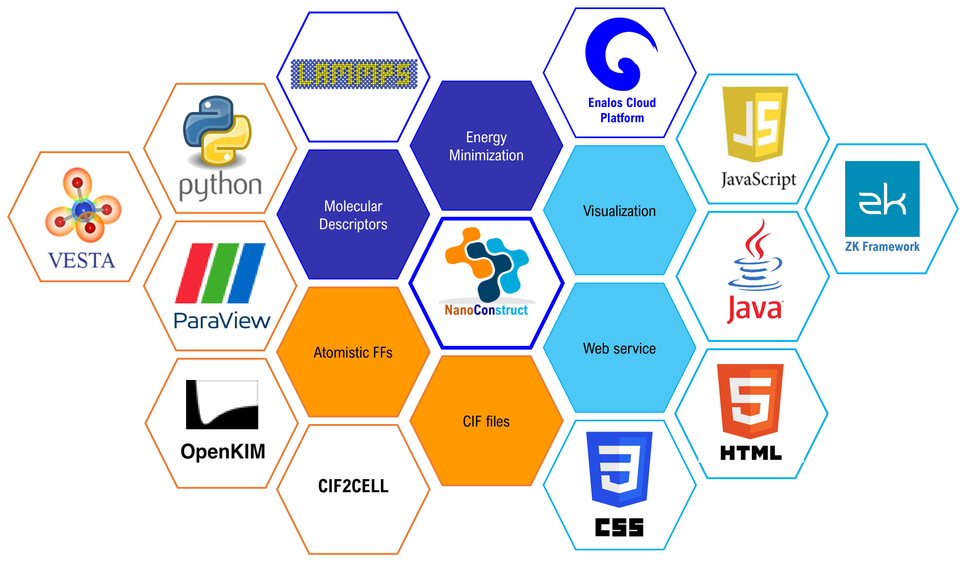
NanoConstruct: A toolbox for the digital reconstruction of Energy Minimized NanoParticles Powered by Enalos Cloud Platform

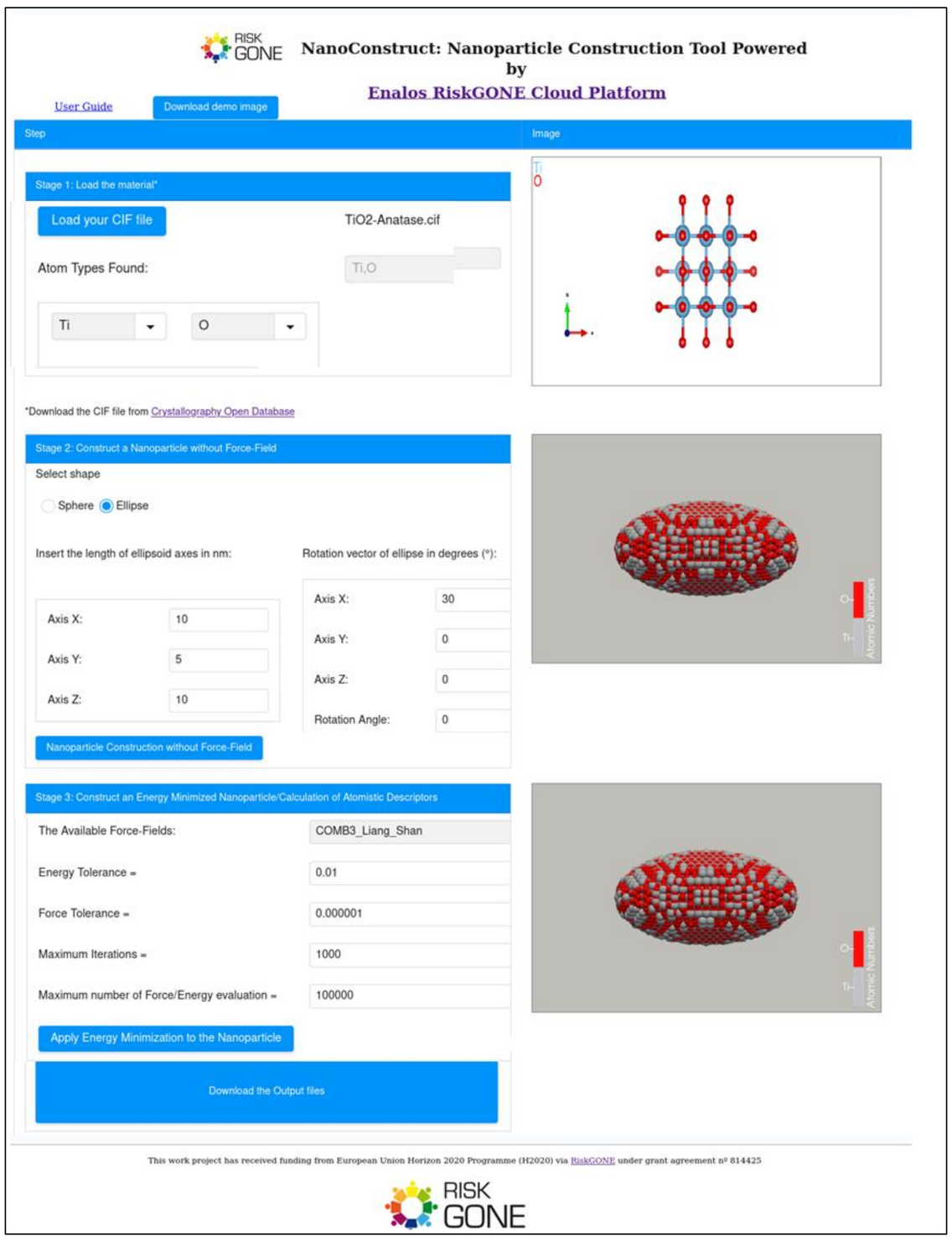
Panagiotis D. Kolokathis[1,2,3], Nikolaos K. Sidiropoulos[1], Andreas Tsoumanis[1,2,3], Kaido Tämm[4], Iseult Lynch[3,5], Antreas Afantitis[1,2,3]
[1]NovaMechanics MIKE, Athens, Greece
[2]NovaMechanics Ltd, Nicosia, Cyprus
[3]Entelos Institute, Larnaca, Cyprus
[4]Institute of Chemistry, University of Tartu, Tartu, Estonia
[5]University of Birmingham, Birmingham, United Kingdom

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) 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.



Input



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.

Output

List of calculated descriptors

descriptors.txt

```
Cif title: Ag.cif
Nanoparticle Diameter: 60.0
Force Field: EAM_Dynamo_AcklandTichyVitek_1987_Ag__MO_212700056563_005
Energy Tolerance: 0.01
Force Tolerance: 1.0E-6
Maximum Iterations: 1000
Maximum number of Force/Energy evaluation: 100000
D1001: Log10 of all atoms in the NP: 3.805908455074197
D1002: Log10 of all atoms in the core: 3.6188844849954505
D1003: Log10 of all atoms in the surface: 3.3498600821923312
D2001: The average potential energy of all atoms in eV is : -2.863655133306969
D2002: The average potential energy of the core atoms in eV is: -2.9542961324791315
D2003: The average potential energy of the shell atoms in eV is: -2.695252419027302
D3001: The average coordination parameter of all atoms is : 11.120075046904315
D3002: The average coordination parameter of the core atoms is: 12.0
D3003: The average coordination parameter of the shell atoms is: 9.485254691689008
D4001: The diameter of the NP in A is: 59.828220009291506
D4002: The surface area of the NP in A^2 is: 11245.066725365388
D4003: The volume of the NP in A^3 is 112128.7210107206
D4004: Lattice energy of NP in eV: -2.863655133306969
D4005: Lattice energy of bulk material - Lattice energy of NP in eV: 0.004181574551219036
D4006: Lattice energy of NP divided by the NP diameter in eV/A: -0.04786462196037647
D4007: Lattice energy of NP divided by the NP surface in eV/A^2: -0.00025465879422906847
D4008: Lattice energy of NP divided by the NP volume in eV/A^3: -2.5538997568991942e-05
D8001: The average CNP of all atoms is : 10.840304261930045
D8002: The average CNP of the core atoms is: 5.726698612789381
D8003: The average CNP of of the shell atoms is: 20.340917438484272
D9001: The average first hex parameter of all atoms is : 0.5294667597769903
D9002: The average first hex parameter of the core atoms is: 0.7999000442903286
D9003: The average first hex parameter of the shell atoms is: 0.027026367906368743
D9004: The average second hex parameter of all atoms is : 2.248787720767763 3e-06
D9005: The average second hex parameter of the core atoms is: 5.817220998355735e-07
D9006: The average second hex parameter of the shell atoms is: 5.346043686734505e-06
```

- data.after_minimization
- data_after_NP_creation.txt
  → lammps datafiles for the minimized and the geometry constructed NP
- descriptors.csv
- descriptors.txt
  → files containing the calculated Descriptors
- Geom_NP.xyz
- lammps.data
  → xyz file of the geometry reconstructed NP
- Minim_NP.xyz
  → xyz file of the minimized reconstructed NP
- Stage1.png
- Stage2.png
- Stage3.png
  → Figures of the unit cell, geometry reconstructed NP and energy minimized NP

This project has received funding from the European Union's Horizon 2020 research and innovation programme under agreement No814425

Antreas AFANTITIS
Managing Director
NovaMechanics Ltd

RiskGONE final Consortium meeting and workshop
Madrid, 15-16 06 2023