The European Nanotechnology Community Informatics Platform: Bridging data and disciplinary gaps for industry and regulators

Nanoinformatics Model for Zeta Potential Prediction Powered by Enalos Cloud Platform

A brief tutorial

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Overview

Online zeta potential predictions for nanoparticles (NPs) are made available through Enalos Cloud Platform, which hosts a fully validated predictive model developed by NovaMechanics Ltd based on a set of indicated properties.

The platform can be easily accessed, there is no need for authorization and the user can directly use the provided service. The web service provides the functionality to virtually screen a set of NPs of interest based on the validated model. Enalos Cloud Platform for NPs aspires to act as a useful aid within a virtual screening framework, for the design of novel NPs.

The tool can be easily accessed through the link:

http://enaloscloud.novamechanics.com/EnalosWebApps/ZetaPotential/

A demonstration video is available at:

https://www.youtube.com/watch?v=swPtFTmI1AI&feature=youtu.be

Instructions

Step 1: Required input

To initiate a prediction, the user must indicate the type of core of the NPs and the pH of the solution where the experimental measurement of the zeta potential would have been made. In addition, the user must provide the value of the main elongation of the NPs. Main elongation is an image descriptor that can be calculated from TEM images using the Enalos NanoXtract tool or another image analysis tool of interest (e.g. ImageJ). The user has two alternative ways to provide the above information either by completing the provided form (Figure 1A) or by importing a .csv file (Figure 1B).

Figure 1: Enalos Zeta Potential Prediction platform. At the top page the input form can be seen and at the bottom by clicking on Upload csv file button, the user can import a .csv file with all the required properties.

Manual entry

For only one entry: Each row corresponds to one NP. The user selects from the first drop-down menu the type of core of the NP (pure metal/oxide) and from the second the pH value (6.5/7) of the medium of interest. Finally, the user enters a numerical value of main elongation between 0 and 1.

For multiple entries: Different rows correspond to many NPs. The user provides information as above and now fills in data for multiple rows each corresponding to one NP. When directly submitting data through the online form, multiple entries are available for up to 20 NPs.

File entry

For one NP or for a set of NPs, all necessary information can be submitted via a .csv file by clicking the **Upload csv file** button. The file must have a specific format (Figure 2) as described below. A template file is also available to download (Figure 1C).

Rows: In the first row the following column names should be included in the specific order: "NP sample", "Type of core", "pH", and "Main Elongation".

Columns: Data should be included in each of the four columns for as many rows as the number of NPs. Column (1): An id is given by the user for his internal use and identification of the NP when results are generated, Column (2): A text is given among two options: "pure metal", and "oxide", Column (3): A numerical value for the pH is given; either 6.5 or 7 and, Column (4): A numerical value for main elongation between 0 and 1 is given.

	A	B	C	D
1	NP sample	Type of core	pH	Main Elongation
2	IO166E Gold 12 nm PEG-OH	pure metal	6.5	0.044918882
3	AgNPs PEG 10nm	pure metal	7	0.031727412
4	AgNPs PEG 20nm	pure metal	7	0.180722892
5	AgNPs PVP 7nm	pure metal	7	0.042328042
6	TiO2 103	oxide	7	0.580700546
7	prom ZnO	oxide	7	0.609965636
8	Ce NM 211	oxide	7	0.019771807
9	S40	pure metal	7	0.043717949
10	IO003	pure metal	6.5	0.017090053

Figure 2: Required format of the .csv file with a sample of input data.

By clicking the **Execute computation** button found under the online form or under the imported .csv file (Figure 1D), depending on the method chosen to provide the input data, predictions for each NP are generated.

Step 2: Output-results

As described above, when properties are uploaded for a set of NPs, a prediction is generated by submitting the input values, the predictive model is then applied to the data provided and the output is generated within seconds (Figure 3).

A table is presented with the produced results. The "Predicted zeta potential [mV]" column contains the zeta potential prediction in mV of each submitted NP, based on the predictive model. The "Reliability" column contains an indication on the reliability of predictions based on the model's domain of applicability limits. Two options are available: The "reliable" option which indicates a prediction within the domain of applicability of the model and the "unreliable" option which is a warning for a prediction out of the domain of applicability of the predictive model.

Row ID	Predicted zeta potential [mV]	Reliability
"IO166E Gold 12 nm PEG-OH"	-0.5815616505801628	"reliable"
"AgNPs PEG 10nm"	-23.554501736363807	"reliable"
"AgNPs PEG 20nm"	-27.79291401386539	"unreliable"
"AgNPs PVP 7nm"	-29.631770892835036	"reliable"
"TiO2 103"	23.107595387224467	"reliable"
"prom ZnO"	18.615889644766884	"reliable"
"Ce NM 211"	38.20268062475627	"reliable"
"S40"	-28.832095935920286	"reliable"
"IO003"	-10.691819408446678	"unreliable"

Figure 3: Generated output page. The first column of the results table contains the prediction for each input NP and the second column contains the reliability of each prediction based on the model's domain of applicability. This table can also be downloaded in .csv and .html format by clicking in the corresponding button.

By clicking the **Download files** button, the above table is downloaded in .csv format. In the downloaded files the neighbors of each particle in the training set can be also found.

If more NPs need to be submitted, the user can return to the initial page and by clicking on the **Reset** button next to **Execute computation** button (Figure 1E) the data are cleared, and new input data can be submitted.

Developed by

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