Case studies on the NanoSolveIT and NanoCommons nanoinformatics models

A. G. Papadiamantis, J. Jänes, E. L. Sikk, J. Burk, P. Burk, A. Tsoumanis, M. K. Ha, T. H. Yoon, E. Valsami-Jones, I., G. Melagraki, K. Tämm and A. Afantitis

This work was funded by:
The EU H2020 project NanoSolveIT (Grant Agreement No. 814572) and the EU H2020 research infrastructure NanoCommons (grant agreement no. 731032) and the POST-DOC/0718/0070 project, co-funded by the European Regional Development Fund and the Republic of Cyprus through the Research and Innovation Foundation,

NSC Education Day
NanoSafe 2020, Nov 2020

ENMs ζ-potential in water

- **The dataset originates from the FP7 NanoMILE project (Joossens et al. 2019)**
- **Enriched with molecular descriptors**
- **Five (5) significant descriptors**:
  - Two (2) **physicochemical** descriptors: **ENM core size and coating**
  - Three (3) **molecular** descriptors: **r_{ion}, $\Sigma\chi/N_O$ and χ_{abs}**
- **Model predictivity: 90.0%**
- **Applicability domain: 1.947**
- The produced model is complemented with a **REST API** to make it available and easy to use programmatically, i.e., to **implement into a workflow**, e.g., in KNIME nodes.
- The model **does not require any experimental measurements** for it to be used and, thus, can be used for the design of new ENMs and in safe by design strategies.

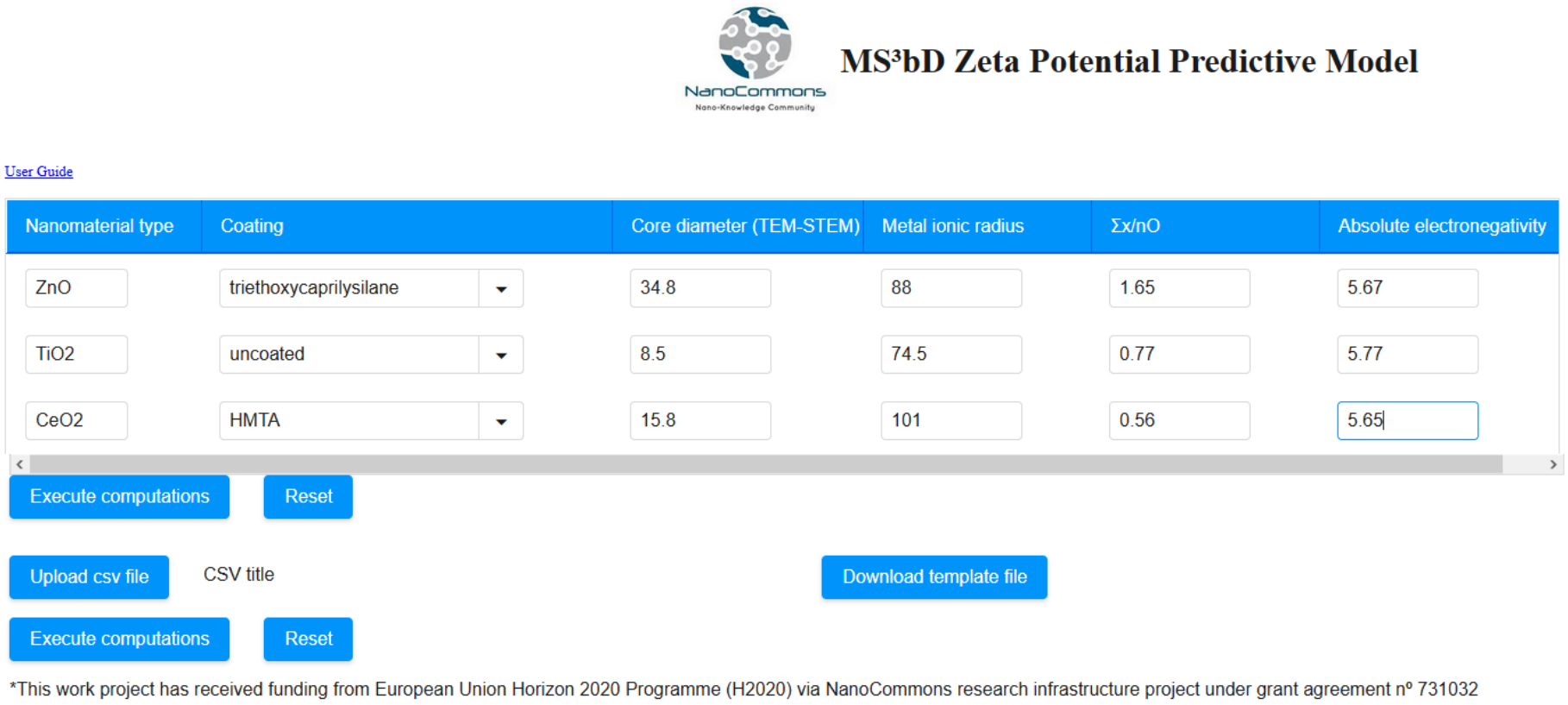
Criterion	Result	Assessment
$R^2 > 0.6$	0.900	Pass
$R_{cvext} > 0.5$	0.913	Pass
$\frac{R^2 - R_0^2}{R^2} < 0.1$	0.005	Pass
$\frac{R^2 - R_0'^2}{R^2} < 0.1$	0.001	Pass
$\lvert R^2 - R_0'^2 \rvert < 0.3$	0.004	Pass
$0.85 < k < 1.15$	1.053	Pass
$0.85 < k' < 1.15$	0.869	Pass

Papadiamantis et al., 2020, Under preparation

User interface

http://enaloscloud.novamechanics.com/nanocommons/mszeta/

Data input



Available coating and capping types: uncoated, Tween 20, sulphate & PVP, Tannic acid / sodium citrate, HMTA, PEG, PEG-1500, Ethylenediamine, PVP, PVP-10K, PVP-40K, PVP-360K, AA4040, D540, aminoacid, aminoalkyl, epoxysilane, sodium citrate, triethoxycaprilysilane

Papadiamantis et al., 2020, Under preparation

User interface

http://enaloscloud.novamechanics.com/nanocommons/mszeta/

Results

Download files

ID	Zeta potential prediction	Closest NN1	Distance from NN1	Closest NN2	Distance from NN2	Closest NN3	Distance from NN3	Closest NN4
ZnO	8.535	CeO2 (PROM)	1.109	CeO2 JRC NM-212	1.112	CeO2-PVP40 (UoB)	1.112	CeO2-PVP10 (UoB)
TiO2	21.250	TiO2 AA4040 (PROM)	0.267	TiO2 JRC NM-103	0.275	TiO2D540 (PROM)	0.309	CuO-PVP360 (UoB)
CeO2	7.689	CeO2 (PROM)	0.061	CeO2 JRC NM-212	1.000	CeO2-PVP40 (UoB)	1.000	CeO2-PVP10 (UoB)

Distance from NN4	Closest NN5	Distance from NN5	Closest NN6	Distance from NN6	Closest NN7	Distance from NN7	APD Prediction
1.113	CeO2_IKR1_ (UoB)	1.113	CeO2_IKS6_ (UoB)	1.113	ZnO-TECS (JRC NM-111) Nanogenotox protocol	1.113	reliable
0.351	CeO2_IKR1_ (UoB)	0.960	CeO2 JRC NM-212	0.961	ZnO-TECS (JRC NM-111) Nanogenotox protocol	1.011	reliable
1.000	CeO2_IKR1_ (UoB)	1.000	CeO2_IKS6_ (UoB)	1.000	CeO2_IKC3 (UoB)	1.001	reliable

Papadiamantis et al., 2020, Under preparation

M_xO_y Cytotoxicity of BEAS-2B and RAW 264.7 cells

- **Dataset retrieved from the S²Nano database (http://portal.s2nano.org/)**
- **Enriched with molecular and atomistic descriptors**
- **Seven (7) significant descriptors**:
  - Two (**2**) **physicochemical** descriptors: **ENM core size** and **hydrodynamic size**
  - Two (**2**) **assay-related** descriptors: **assay type (ATP or LDH)** and **exposure dose (μg/mL)**
  - Three (3) **molecular/atomistic** descriptors: ***E_C*, the coordination number of metal atoms in the shell region and the force vector surface normal component of atoms (metals and oxygens) in the shell region**
- **Model predictivity: 91.0%**
- **Applicability domain: 2.645**
- The produced model is complemented with a **REST API** to make it available and easy to use programmatically, i.e., to **implement into a workflow**, e.g., in KNIME nodes.

Criterion	Result	Assessment
$R^2 > 0.6$	0.910	Pass
$R_{cvext} > 0.5$	0.904	Pass
$\frac{R^2 - R_0^2}{R^2} < 0.1$	0.022	Pass
$\frac{R^2 - R_0'^2}{R^2} < 0.1$	0.002	Pass
$\lvert R^2 - R_0'^2 \rvert < 0.3$	0.018	Pass
$0.85 < k < 1.15$	0.994	Pass
$0.85 < k' < 1.15$	1.005	Pass

Papadiamantis et al., Nanomaterials 2020, 10(10), 2017

User interface

https://cellviability.cloud.nanosolveit.eu/2/

Data input

NanoSolveIT Cloud Platform

NanoSolveIT Cytotoxicity (Cell Viability) Prediction for Metal Oxide NPs

User Guide

User row ID	Core size (nm)	Hydro size (nm)	Ec (eV)	Assay	Exp. dose (ug/mL)	Coord. #Me atoms	V⊥ #all atoms
CuO	25	45	-5.17	ATP	3.2	3.579	-0.243
CeO2	64	120	-3.8	LDH	0.8	7.011	-1.108
HfO2	14	78	-2.96	ATP	200	6.215	-0.924
ZnO	89	92	-3.89	ATP	50	3.586	0.868
SiO2	73	134	-2.02	LDH	15	3.644	-1.162

Results

Download files

ID	APD Prediction	kNN Prediction	Closest NN1	Distance from NN	Closest NN2	Distance from NN	Closest NN3	Distance from NN	Closest NN4	Distance from NN
CuO	reliable	1.6576248278753	ZnO	2.2228655489475	ZnO	2.2232594323735	ZnO	2.2275501962159	ZnO	2.2491214514422
CeO2	reliable	1.9480636756013	In2O3	2.6343319087030	In2O3	2.6343620830066	In2O3	2.6346034649939	In2O3	2.6357577383235
HfO2	reliable	1.9494421379711	La2O3	1.6744372048920	La2O3	2.2995194093385	NiO	2.5362383156147	SiO2	2.6053928616888
ZnO	unreliable	1.8548693934997	CoO	2.7147474904932	CoO	2.7431928540824	CoO	2.7783400451756	CoO	2.8131691040787
SiO2	unreliable	1.9786340403035	Gd2O3	2.8756779807982	Gd2O3	2.8791121804392	Gd2O3	2.8800645355588	Gd2O3	2.8805612914982

Papadiamantis et al., Nanomaterials 2020, 10(10), 2017

NanoSolveIT

NanoCommons
Nano-Knowledge Community

This work was funded by:
The EU H2020 project NanoSolveIT (Grant Agreement No. 814572) and
the EU H2020 research infrastructure NanoCommons (grant agreement no. 731032) and
the POST-DOC/0718/0070 project, co-funded by the European Regional Development Fund
and the Republic of Cyprus through the Research and Innovation Foundation,