NanoSafety Cluster

Nanosafety Cluster Review

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EU Networking and Community Building

WG6 - Modeling

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Scope & Objectives

- Computational modeling for nanoEHS
  - NP models (structure, **<u>properties</u>**, descriptors)
  - NP behavior models (exposure, **<u>hazard</u>**)
  - Risk models
  - Decision – making
- **Objectives**
  - ST: Communication strategy between projects
  - MT: Inventory of published models, reference dataset for model validation
  - LT: Guidelines for QNPR/QNAR development and validation

Context

- Interaction with all NSC WGs, specifically:
  - WG4, WG5 and WG8
- Harmonization of FP7 NMP Modeling projects
  – Nanodescriptors and QSAR WG
- MODENA COST Action (Modelling Nanomaterial Toxicity, TD1204)
- US-EU CoRs
  - Predictive Modeling for Human Health

Communication Strategy & Activities

- Mostly face-to-face
  - WG sessions in NSC Meetings and other international events (e.g. Young Scientist a Forum)
- Coordination activities to minimize overlap and to create synergies
  - US-EU Communities of Research
  - Harmonization of NMP modeling projects
  - WGs in MODENA
- 2015 - ...
  - Webinar series in collaboration with the above initiatives

WG Deliverables (2015)

- <u>Inventory of models</u> as a first step towards the establishment of a model repository to facilitate sharing, reuse and cross-validation (in coordination with eNanoMapper)
- <u>Reference dataset</u> for model validation and comparative performance analysis
- <u>Guidelines</u> for model development, validation and reporting
- Springer book on Computational Modeling (Tran, Bañares, Rallo eds., 2015)

Expected impact

- The establishment of systematic guidelines for model development and validation will facilitate the generation of **robust predictive models** that will contribute to the implementation of risk assessment, intelligent testing strategies and ultimately, to a new generation of safe-by-design nanomaterials.

Future activities

- Shift the focus from structure-property/activity relationships to a wider spectrum of modeling techniques
- Foster the creation of specific interest groups to expand the activities to other computational modeling approaches relevant for nanoEHS