



# Nanosafety Cluster Meeting

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WG6 - Modeling. Progress Report

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# Scope & Objectives

- **Scope:** Computational modeling for nanoEHS
  - NP models (structure, properties, descriptors)
  - NP behavior models (exposure, hazard)
  - Risk models
  - Decision - making
- **Objectives**
  - Facilitate the coordination with ongoing initiatives
  - Foster sustainability of research results beyond project's life

# Coordination with ongoing initiatives

- **Internal:**
  - Other NSC WGs, specifically:
    - WG4, WG5 and WG8
  - EU Projects:
    - FP7 NMP Modeling projects, H2020 Projects
    - COST Actions (e.g., MODENA)
  - European Materials Modeling Council (EMMC)
- **External:**
  - US-EU CoRs

# Dissemination & Sustainability of research results

- Inventory of models and tools to facilitate sharing, reuse and cross-validation (coordinated by eNanoMapper)
- Reference dataset for model validation and comparative performance analysis
- Guidelines for model development, validation and reporting
- Springer book on Computational Modeling (Tran, Bañares, Rallo eds., 2016)

# Future activities/needs

- New leadership after the end of FP7 projects
- Alignment of NSC WGs with the US-EU CoR structure
  - Proposal: integration of WG4 & WG6
- Collaboration with EMMC
  - Use of physics & chemistry based models in nanosafety
  - Preliminary document: Materials Modeling for Toxicity
    - [http://emmc.info/wp-content/uploads/2016/05/MaterialsModelling-for-Nanotoxicity\\_2016-05-16\\_v08.pdf](http://emmc.info/wp-content/uploads/2016/05/MaterialsModelling-for-Nanotoxicity_2016-05-16_v08.pdf)