



14 Giugno 2019
alle ore 11.00

presso AULA 1 dell'Edificio F
Area della Ricerca CNR
Via Madonna del Piano, 10 Sesto Fiorentino (Firenze)

Dr. **Felice C. Simeone**

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terrà il seguente seminario:

**" Anticipating the Toxicity of Oxide Nanoparticles with just a
Periodic Table "**

Si invitano tutti gli interessati a partecipare.

Dr. Alessandro Lavacchi
Ricercatore ICCOM

Dr. Francesco Vizza
Direttore ICCOM

Short Abstract:

The current frenzy in the development of new nanomaterials calls for continuous evaluations of the risks they pose; non-experimental assessments of potential hazards would expedite decision processes to safeguard consumers, workers, and the environment. We show that the toxicity of nano-oxides can be anticipated on the basis of a series of physical-chemical parameters that capture fundamental aspects of the chemistry of the nanoparticles and whose quantification does not involve complex modeling or time-consuming experiments, because they can be retrieved from a periodic table. Combining these parameters in a naïve Bayes classifier, a robust probabilistic model that can be run on a pocket calculator, makes it possible to determine the most probable level of toxicity of a nanoparticle given its composition. Results indicate that toxicity of nano-oxides decreases with the oxidation number (Z) of the cation; high values of Z , however, may become unstable and activate adverse redox processes. By contrast, stable reducible oxides tend to be, probabilistically, less toxic than oxidizable ones.

Biographic sketch **Felice C. Simeone** studied chemistry in Florence. He received a PhD in nano-electrochemistry from the University of Ulm-Germany, where he worked in the group of Prof. Kolb. He was a Post-Doctoral Fellow in the G. M. Whitesides' group at the Dep. Of Chemistry and Chemical Biology of Harvard University-USA. Before joining the CNR in Faenza, he was a Senior scientist at Wageningen University-The Netherland. Over the years, he conducted research in nano-chemistry for applications in fields as diverse as electro-catalysis, molecular electronics, and nanosafety.