



# ITE/IEXMH

## ΣΕΜΙΝΑΡΙΟ ΣΕΜΙΝΑΡΙΟ

**ΟΜΙΛΗΤΡΙΑ:** **Eirini Goudeli**, Post-Doctoral Fellow  
Department of Mechanical Engineering  
University of Minnesota, USA

**ΘΕΜΑ:** **Multiscale Design of Aerosol Synthesis of Nanomaterials**

**ΤΟΠΟΣ:** Αίθουσα Σεμιναρίων ITE/IEXMH

**ΗΜΕΡΟΜΗΝΙΑ:** **Πέμπτη, 8 Ιουνίου 2017**

**ΩΡΑ:** **16:00**

### ΠΕΡΙΛΗΨΗ

Nanoparticles have attracted strong interest due to their novel properties and have been explored widely in photonics, electronics, catalysis, sensors and information storage. Gas-phase methods, such as flame reactors, are used routinely for commercial synthesis of nanostructured particles (e.g. fumed silica, pigmentary titania, carbon black, Ni) as well as for advanced materials (e.g. photocatalysts, nanofluids and biomaterials). Such nanostructured commodities consist of clusters of primary particles (PPs) that are formed by chemical reactions, condensation/evaporation or surface growth and grow further by sintering and coagulation. Depending on process conditions, gas-phase synthesis typically results in aggregates (highly-sintered particles) which are attractive in catalysis, lightguide preforms and electronics and, downstream in the process in agglomerates (PPs held together by rather weak, physical forces) that are attractive in nanocomposites, pigments and liquid suspensions. The dynamics of aerosol reactors and product nanoparticle characteristics span 10 and 15 orders of magnitude in length and time requiring different models for each scale. In this talk, multiscale design of aerosol reactors for synthesis of nanomaterials will be discussed, focusing on recent advances in aerosol particle formation, crystalline structure and



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process design optimization. More specifically, Molecular Dynamics (MD) simulations are used for the accurate quantification of small (below 10 nm) nanoparticle sintering rates and crystallinity dynamics. Even though progress in particle synthesis has allowed close control of collision and sintering rates, crystallinity is controlled rather empirically in practice (e.g. by the use of dopants). Crystalline structure plays crucial role in electronics as it affects transport properties and in catalysis where high-index facets enhance catalytic activity. Mesoscale models provide the transport properties (diffusion, settling rates, etc.) and interaction (coagulation rate) of multi-particle structures. Discrete Element Modeling (DEM) is used here to track the detailed structure and size distribution of fractal-like agglomerates. Easy-to-use relations are derived that can be readily interfaced with climate dynamics, meteorological models or computational fluid dynamics describing the reactor operation and particle production. Interfacing the above models can facilitate the understanding and design of aerosol reactors for synthesis of nanoparticles whose properties can be closely controlled during scale-up from laboratory scale to commercial products. This systematic approach to study particle formation can offer significant insight into fundamental physical principles and mechanisms that may be exploited by chemical industry and nanotechnology.

## **ΣΥΝΤΟΜΟ ΒΙΟΓΡΑΦΙΚΟ**

Eirini Goudeli is Post-doctoral Fellow at the Department of Mechanical Engineering, University of Minnesota. After receiving her Diploma in Chemical Engineering in 2012 from University of Patras, Greece, she joined the Particle Technology Laboratory at ETH Zurich and earned her PhD in 2016. She received a best poster award at the 2013 European Aerosol Conference in Prague, CZ, September 1 – 6, a best presentation award by a PhD student at the 2014 Symposium HH on Flame and High-Temperature Synthesis of Functional Nanomaterials during the Fall meeting of the Materials Research Society, Dec. 1-4, Boston, USA and a 3rd best poster award at the 2015 Particle Technology Forum Poster Session, AIChE Annual Meeting, November 8 – 13, Salt Lake City, UT, USA. In 2016, she received the ETH Medal for Outstanding PhD Thesis.