



ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ

ΣΧΟΛΗ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

ΔΙΑΛΕΞΗ

Graduate Research at the Interface between Computational Materials Science and Traditional Chemical Engineering

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Περίληψη

Overcoming the pressing technological challenges of 21st century requires a synergistic approach, combining fundamental research with advanced engineering. Adopting this principle, the Chemical Engineering Department at UCL offers unique opportunities to aspiring graduate students, by providing a diverse environment nurturing innovative developments. In the first part of this talk we will therefore discuss these opportunities, touching upon the breadth of research performed at this Department. Subsequently, in the second part, we will focus on the latest developments from the Multiscale Computational Catalysis and Materials Science lab, led by the seminar speaker. These developments have led to computational methodologies and open source software for assessing the performance of catalytic materials towards reactions of practical importance. The materials discovered and validated through collaborations with experimentalists and industry, are expected to change the technological landscape for processes such as methane or CO₂ conversion to fuels, emissions control, or biomass valorisation.