

NOMATEN HYBRID-SEMINAR

<https://www.gotomeet.me/NCBJmeetings/nomaten-seminar>

In-person: PNT Maria seminar room

Tuesday, FEBRUARY 14st 2023 13:00 CET

Strategies for materials design from atomistic simulations

Dr. Javier LLorca

IMDEA Materials Institute & Polytechnic University of Madrid, Spain.

Abstract: The ever increasing power of digital computers and the maturity of atomistic simulation tools based on first principles calculations and molecular mechanics provide a unique opportunity to design new materials for engineering applications in silico. The main limitation is often found in the need to deal with much larger length scales and longer time scales than those allowed by atomistic simulations and, thus, novel strategies are required.

In this talk, several strategies to design materials from atomistic simulations for various engineering applications are reviewed. They include the predictions of phase diagrams of different alloys of technological interest from first principles calculations and statistical mechanics including the effect of configurational and vibrational entropy as well as magnetism, the simulation of precipitation hardening due to the interaction of dislocations with Guinier-Preston zones in Al-Cu alloys as well as the search for new intermetallic catalysts for the hydrogen evolution reaction and the oxygen reduction reaction from first principles simulations and machine learning tools.

Bio: Prof. Javier LLorca earned his BEng/MSc in Civil Engineering with honors from the Technical University of Madrid in 1983, followed by his PhD in Materials Science from the same institution in 1986. He then went on to become an Associate Professor in the Department of Materials Science at the Technical University of Madrid in 1987, and was promoted to full Professor in 1995. Since 2006, he has been the head of the research group on “Advanced Structural Materials and Nanomaterials”. In 2007, he founded the IMDEA Materials Institute and served as its director until 2017, when he became the Scientific Director. Prof. LLorca has received numerous awards, including the Research Award from the Spanish Royal Academy of Sciences, the Research award from the Technical University of Madrid, and the Career Award from the Spanish Society of Materials (SOCIEMAT).

Currently, Prof. LLorca is the Executive Editor of Modelling and Simulation in Materials Science and Engineering, and an editor of Materials Research Letters. He is also an Associate Editor of multiple journals, including Composites Science and Technology, Materials Science and Engineering A, International Journal of Multiscale Computational Engineering, Integrating Materials and Manufacturing Innovation, and International Journal of Engineering Sciences and Advanced Theory and Simulation. In addition, he chairs the European Mechanics of Materials Conference Committee.



institute
imdea
materials

