ENERGETICS

Ateneo/Denerg - MULTI-scale modeling of thermophysical, mechanical and wetting properties of high ENTROPY alloys for energy applications(MULTIENTROPY)

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Context of the research activity	The MULTIENTROPY project aims at a rational design framework, integrating multi-scale computational modeling (from electronic to continuum scale) with high-throughput synthesis and characterization, to optimize High-Entropy Alloy (HEA) performance and safety. By coupling physical models with advanced machine learning techniques, MULTIENTROPY accelerates material innovation, ensuring these novel coatings contribute to a sustainable future in energy, manufacturing, and transportation.
Objectives	High-entropy alloy (HEA) coatings are next-generation materials aim to replace traditional, toxic, and rare materials with sustainable alternatives that are free from rare earths and reduce the use of critical raw materials (CRMs) by 30-40%. HEAs offer exceptional thermophysical, mechanical, and wetting properties, such as high thermal conduction, low friction, high strength, and corrosion resistance, making them ideal for energy-related applications. Innovative coatings based on HEA can significantly improve the functionality of technologies in renewable energy production (e.g. wind turbines), storage (e.g. electrodes for batteries), aerospace (e.g. turbine blades), and automotive (e.g. engine parts) sectors. The PhD research project addresses the development of next-generation coatings based on HEA through multi-scale, data-driven computational modeling. The work will focus on simulation, supported by AI/ML tools, of the thermophysical, mechanical and wettability properties of such HEA coatings, with the goal of driving the synthesis process toward optimal conditions. We approach this through a sequence of steps: 1. Development of selected HEA simulation domains with classical force fields available in the literature (6 months). 2. Assessment of thermophysical (e.g. thermal conductivity, heat capacity, density, friction coefficient), mechanical (e.g. elastic moduli), and wetting (e.g. surface free energy, contact angle) properties of HEA by classical Molecular Dynamics – MD (12 months).

	3. Training and implementation of reactive force-field of HEA bulk and surface domains, informed by datasets from electronic simulations by the University of Birmingham, to include relevant reactive mechanisms into the activities #1 and #2 (12 months). 4. Simulation upscaling and validation, in collaboration with the University of Strathclyde and the National Technical University of Athens (6 months). The PhD activity will be carried out mainly at the Multi-Scale modeling Laboratory at the Energy Department of Politecnico di Torino, in close collaboration with the University of Birmingham (UK, electronic modelling), the University of Strathclyde (UK, meso- and macroscopic modelling), and the National Technical University of Athens (Greece, experimental validation).

Skills and competencies for the development of the activity	• Proficiency in thermodynamics and heat and mass transfer phenomena. • Expertise in atomistic simulations and high-performance computing (HPC) systems. • Understanding of nanoscale heat and mass transport mechanisms, as well as the thermal, mechanical, and wettability properties of surfaces. • Knowledge of statistical thermodynamics and experience with the development and application of computational models would be a plus.