Dario Marrochelli
Research Scientist,
Nuclear Science & Engineering
MIT

Host: Ming Su
m.su@neu.edu

"From First-Principles to Renewable Energy"

Monday, January 26
346 Curry
11:45 a.m. – 1:00 p.m.

Refreshments will be served

ABSTRACT The greatest challenge of our time is to generate and store energy in a sustainable manner. While we have many promising technologies that can generate (e.g. wind, solar, fuel cells) and store (e.g. Li-ion batteries, electrolyzer cells) renewable energy, these are expensive, intermittent and unreliable. Materials are the common bottleneck of all these technologies. The challenge, therefore, becomes finding advanced materials that deliver higher performance and reliability, while being affordable and environmentally friendly. Nowadays, it takes between 10-20 years to incorporate new materials into applications. The traditional material science approach of trial-and-error is too slow and the challenges we are facing in the field of renewable energy need faster solutions. This can only be achieved with a paradigm-shift approach to materials science, in which the trial-and-error method is substituted by the rational design of materials through computer simulations. In this presentation, I will review some of my recent research combining computation and experimentation to rationally design new materials. I will provide three examples: first, I will talk about chemical expansion in oxide materials, a detrimental property that affects the performance of solid oxide fuel cells and batteries. I will show how we understood the atomistic causes of this phenomenon and predicted materials with reduced expansion. Second, I will focus on the oxide-ion conductivity, a key figure of merit of electrolyte materials for solid oxide fuel cells, and discuss possible routes to enhance this property. Third, I will present our latest work on the role of dislocations on the defect chemistry and oxide-ion mobility in $SrTiO_3$, and discuss its implication for resistive switching memories.

BIOGRAPHY Dario Marrocchelli (https://marrocchelli.mit.edu/) is a Research Scientist at MIT, working at the Laboratory for Electrochemical Interfaces. The goal of his research is to obtain better renewable energy technologies by designing advanced materials with higher performance, through computer modeling. Dario also worked as a postdoctoral associate at Trinity College Dublin (2011-2013) and MIT (2010-2011). He did his doctoral work at the University of Edinburgh under the supervision of Professor Paul Madden (2006-2010). Dario has been awarded several honors, including a Marie-Curie postdoctoral fellowship and has raised $1,000,000 in funds during his career. His work has been published in 30 journal papers (including *Nature Communications, Advanced Functional Materials and Energy and Environmental Science*) and one book chapter, with a total of 580+ citations and an h-index of 15. Dario served as guest editor of a special issue on Electro-Chemo-Mechanics of the Journal of Electroceramics and is currently editing a book on the same subject for Springer. He also greatly enjoys teaching and he has recently developed and delivered a course on the Science of Cooking.