

JOINT SEMINAR

Texas Center for Superconductivity at the Univ. of Houston
Materials Engineering Program
Center for Integrated Bio and Nano Systems

Prof. Pieremanuele Canepa

Department of Electrical and Computer
Engineering, University of Houston

Thursday, May 15, 2025

12:00 p.m. – 1:00 p.m.
Houston Science Center (HSC), 102

Sandwiches provided, first come first served.

How can I get the best out of first-principles simulations for materials predictions?



ABSTRACT: In an era where everybody “runs simulations” in their backyard, responsible choices must be made. In this “experimental” talk, I will review some foundational principles of *ab initio* thermodynamics. What is a phase diagram at 0 Kelvin, aka the convex hull? How do I read a convex hull? Why is a convex hull a handy plot even at tremendously low temperatures, i.e., 0 Kelvin? Can I use the convex hull construction of a pseudo-binary tie-line to understand portions of complex multidimensional phase fields? And many other questions. In the second part of my talk, I will discuss the challenges of using plain vanilla density functional theory to describe every possible material system. What are the risks in doing so?

What should I be aware of? I will connect thermodynamics with first-principles approaches in a hopefully digestible manner.

BIO: Dr. Pieremanuele Canepa is an Assistant Professor in the Department of Electrical and Computer Engineering at the University of Houston. He was a Postdoctoral fellow under the guidance of Prof. Gerbrand Ceder initially at the Massachusetts Institute of Technology and later at Lawrence Berkeley National Laboratory. He received his bachelor's and master's degrees in Chemistry from the University of Torino (Italy) and his Ph.D. from the University of Kent (United Kingdom). His research contributes to the rational design of new materials for clean energy technologies, such as electrode materials for batteries, ionic conductors, and liquid electrolytes for sustainable energy storage devices. In March 2020, Pieremanuele was awarded the National Research Fellowship, equivalent to NSF CAREER in the US. In 2021, Pieremanuele was elected Fellow of the Royal Society of Chemistry, and, in 2022 a Materials Au Rising Star from the American Chemical Society. In 2023, Pieremanuele became a Scialog® fellow.