UCSD NanoEngineering/Chemical Engineering
SPECIAL SEMINAR
Thursday, November 14, 2019
Seminar Presentation: 1:00pm – 2:00pm
SME room 248

"How Data-Science Methods can Accelerate Energy-Materials RD&D: Perspective of a PV Materials Researcher"

Tonio Buonassisi Ph.D.
Professor of Mechanical Engineering
Massachusetts Institute of Technology

Abstract: From the perspective of a photovoltaics materials engineer, I'll summarize my team's last 6 years of research applying advanced statistics and machine-learning algorithms to accelerate three essential materials R&D tasks: **diagnosis**, **process optimization**, and **discovery**. "Diagnosis" refers to the purposeful application of characterization to identify underlying performance limitations, an essential step toward improving early-stage prototypes. As examples of how data science can increase diagnosis speed and efficiency, I'll demonstrate how Bayesian inference enables 10x faster root-cause diagnosis of under-performing early-stage photovoltaic devices, and convolutional neural networks enable 40x faster and interpretable classification of X-ray diffraction spectra. Accurate diagnosis directs "process optimization," which can help determine the performance ceiling of novel materials, and when to abandon unsuccessful candidates quickly. I'll demonstrate how a Bayesian network helps identify new process windows beyond conventional "design of experiments." Lastly, materials screening, in combination with high-throughput experimentation enabled by ML, can enable novel materials "discovery," as we illustrate with the case of novel lead-free perovskite-inspired photovoltaic materials with promising optoelectronic properties, and link these findings to other material systems from the AMDM programme. Themes of "small data sets," "embedded physics," "complexity," "efficient manifold sampling strategies," "data representation," and "transfer learning" generalize to other systems, and promise to accelerate the cycle of learning by $\geq$10x across a range of chemistry and materials disciplines. I'll also highlight educational opportunities and challenges of a new generation of researchers who are highly skilled in both materials and data sciences.

Biosketch: Tonio Buonassisi is a Professor of Mechanical Engineering at the Massachusetts Institute of Technology (MIT). He is pioneering the application of artificial intelligence to develop new materials for societally beneficial applications. His research in solar photovoltaics and technoeconomic analysis assisted technology developments in dozens of companies, earning him a US Presidential Early Career Award for Scientists and Engineers (PECASE), a National Science Foundation CAREER Award, and a Google Faculty Award. He founded the MIT PVLab and co-founded the Fraunhofer Center for Sustainable Energy Systems in Boston USA. A recipient of the prestigious MIT Everett Moore Baker Memorial Award for Excellence in Undergraduate Teaching, his passion for education is evidenced by the >179k views of his OpenCourseware/YouTube PV lectures series, and a recent datasci-focused YouTube video series "Accelerated Materials Development for Manufacturing." He's the founding director of the A*STAR Accelerated Materials Development for Manufacturing programme.