

# Multi-Scale Systems Analytics for Energy and Environmental Sustainability

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## Abstract:

Energy and environmental sustainability have risen to the top of the public and policy agenda, as demonstrated by the recent Glasgow Climate Pact and the rapid proliferation of carbon neutrality pledges across various countries and sectors. Process systems engineering (PSE) theory, methods, and tools play an important role in the quest for energy and environmental sustainability. Combined with chemical and biomolecular engineering domain knowledge, PSE is empowered with the multi-scale feature to investigate scientific problems from nano- to mega-scales. These PSE methodologies organically integrate systems-level analysis, design, control, and optimization theory with modern artificial intelligence techniques for data analytics and machine learning to leverage the power of big data. This talk will illustrate the concepts and methods of multi-scale systems analytics through our research efforts in the areas of sustainable energy technologies and systems, circular economy and food-energy-water-waste nexus, smart technologies for sustainable built environments and food production, and environmental impact and climate change mitigation. Specific examples include our collaborative works with experimentalists and domain experts on (a) integrated design of metal-organic frameworks (MOFs) and adsorption processes via rapid, in-silico screening of MOFs for economically-efficient post-combustion CO<sub>2</sub> capture and separation; (b) effective detection of microplastics in the aqueous environment by developing intelligent soft sensors based on explainable deep learning techniques to analyze complex spatiotemporal optical responses of liquid crystal; (c) quantum computing-assisted deep learning models and algorithms for sustainable and safe operations of electric power systems with renewable energy resources; (d) multi-scale optimization combined with machine learning for the design of 100% renewable energy systems toward carbon neutrality for Cornell University campus and New York State; and (e) climate implications of shifting in-person events to online/hybrid format. The presentation will conclude with a brief overview of multi-scale applications of systems analytics technologies and methods on perovskite photovoltaics, battery second-life, shale gas, biofuels, and CO<sub>2</sub> utilization that range from molecular and materials systems to macro-scale systems, including devices, manufacturing processes, infrastructure, and global climate change.

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# Short CV

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Fengqi You is the Roxanne E. and Michael J. Zak Professor in the Smith School of Chemical and Biomolecular Engineering at Cornell University. He also serves as Chair of Ph.D. Studies in Cornell Systems Engineering, Associate Director of Cornell Energy Systems Institute, and Associate Director of Cornell Institute for Digital Agriculture. His research focuses on fundamental theory and methods in systems engineering and artificial intelligence, as well as their applications to smart manufacturing, digital agriculture, quantum computing, energy systems, and sustainability. His recent awards (in the past six years) include NSF CAREER Award (2016), AIChE Environmental Division Early Career Award (2017), AIChE Research Excellence in Sustainable Engineering Award (2017), Computing and Systems Technology (CAST) Outstanding Young Researcher Award from AIChE (2018), Cornell Engineering Research Excellence Award (2018), ACS Sustainable Chemistry & Engineering Lectureship Award (2018), AIChE Excellence in Process Development Research Award (2019), AIChE Innovations in Green Process Engineering Award (2020), Mr. & Mrs. Richard F. Tucker Excellence in Teaching Award (2020), Curtis W. McGraw Research Award from American Society for Engineering Education (ASEE) (2020), American Automatic Control Council (AACC) O. Hugo Schuck Award (2020), AIChE Sustainable Engineering Forum Education Award (2021), AIChE George Lappin Award (2022), and Stratis V. Sotirchos Lectureship Award by Foundation for Research & Technology – Hellas (FORTH) (2022), in addition to a number of best paper awards. Fengqi is an elected Fellow of the Royal Society of Chemistry (FRSC) and Fellow of the American Institute of Chemical Engineers (AIChE Fellow).

For more information about his research group: [www.peese.org](http://www.peese.org)