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"Harnessing AI for Metallic Glass Innovation: Bridging Structure and Properties"

PAULO BRANICIO

Associate Professor, Chemical Engineering and Materials Science
University of Southern California

Bio: Paulo Branicio is an Associate Professor in the Mork Family Department of Chemical Engineering and Materials Science at the University of Southern California (USC), where he leads the Branicio Research Lab. After earning his Ph.D. in Physics from the Federal University of São Carlos (UFSCar), Brazil, and completing postdoctoral appointments at Louisiana State University and USC, he established himself as a leading researcher at the Institute of High Performance Computing (IHPC) – A*STAR, Singapore, where he served as an Independent Investigator, Scientist, and Senior Scientist from 2008 to 2016. He joined USC as an Assistant Professor in 2017 and was promoted to Associate Professor with tenure in 2024. His research focuses on computational materials science, particularly the applications of machine learning to materials discovery and design, atomistic modeling of metallic glasses and nanoglasses, and the development of scalable parallel algorithms for data mining and structure analysis. His work encompasses nanostructured, heterogeneous, and nanoporous materials, as well as the behavior of metals and ceramics under extreme conditions. With over 104 peer-reviewed publications and a position on the editorial board of Scientific Reports, his contributions continue to advance the frontiers of materials science and engineering.

Abstract: At the intersection of artificial intelligence and materials science, our group is pioneering novel approaches to understand and engineer metallic glasses at the nanoscale. Through innovative AI-driven methodologies, we have made significant advances in three key areas. First, we have employed genetic programming algorithms to establish new predictive models for mechanical properties of nanoporous metallic glasses, enabling accurate property predictions across diverse compositions and architectures. Second, we have leveraged machine learning to uncover previously unknown vacancy-like structural motifs in metallic glasses, demonstrating how AI can reveal hidden structural features that control material behavior. Third, we have developed advanced graph convolutional neural networks that can distinguish subtle structural differences in metallic glass states, achieving remarkable classification accuracies that surpass traditional analytical methods. These advances demonstrate how the convergence of AI and nanoscale materials characterization can accelerate materials discovery and design, moving beyond traditional trial-and-error approaches to enable more targeted development of next-generation materials.