Department of Electrical and Computer Engineering
Materials Engineering Program
Texas Center for Superconductivity at Univ. of Houston
Center for Integrated Bio and Nano Systems
10:00 a.m., April 8, 2022
Join Zoom Meeting
https://zoom.us/j/845619943?pwd=QlZvYUV6M2dxNDkvNWxBd3F2YzdJZz09

Meeting ID: 845 619 943
Password: 016104

Energy Loss Spectroscopy at High Resolution: Probing the local electronic structure and the plasmonic response of materials

Gianluigi Botton

Department of Materials Science and Engineering
McMaster University, Hamilton, ON, L8S 4M1, Canada
Canadian Light Source, Saskatoon, Saskatchewan, Canada

Abstract:

Advances in both experimental and computational methods have dramatically accelerated the prediction, optimization, and validation of organic chemical and materials properties. Despite this progress, chemical stability, which is central to analyzing the life-performance and feasibility of novel organic materials, remains beyond our current capability to predict. This capability gap has resulted in many computational design efforts yielding libraries of conceptually interesting organic molecules and materials that nevertheless often fail to connect with real applications. Moreover, chemical stability prediction faces the challenge that degradation chemistry is poorly represented in reaction databases, and as such cannot use domain heuristics that have been successful in other reaction prediction contexts. In this talk, I'll discuss how recent developments in automated reaction prediction, by our group and others, have created an opportunity to bring chemical stability into the realm of routine predictability. In particular, we have recently been able to reduce the cost of predicting reactions involving generic organic molecules over 100-fold while also improving the accuracy of transition states and increasing the scope of kinetically relevant pathways. This method has been used to elucidate several reaction networks governing thermal degradation. Each of these networks constitutes the most comprehensive exploration to date and all have been generated without using reaction templates or other domain knowledge implements that are commonly used in network construction. On the horizon, the throughput enabled by these and similar efforts will generate valuable data sources for nascent machine learning efforts in this space, which will ultimately allow us to routinely predict how things fall apart.

Short Bio:
Gianluigi Botton received a degree in Engineering Physics and a PhD in Materials Engineering from Ecole Polytechnique of Montréal. He was Postdoctoral Fellow in the Department of Materials Science and Metallurgy at the University of Cambridge from 1993 to 1998. He joined the Materials Technology Laboratory of Natural Resources Canada (NRCan) in 1998 as a research scientist. In 2001 he moved to the Department of Materials Science and Engineering at McMaster University where he holds a Tier 1 Canada Research Chair in Electron Microscopy of Nanoscale Materials. He received the Metal Physics Medal of the Canadian Materials Science Conference (2017), the Lee Hsun Research Award from the Institute Metals Research of the Chinese Academy of Sciences (2017), the Microbeam Analysis Society Presidential Award (2020) and he is Fellow of the Microscopy Society of America and Fellow of the Royal Society of Canada. Prof. Botton established the Canadian Centre for Electron Microscopy-CCEM, a national facility for ultrahigh-resolution microscopy, and was its director for over 11 years. In May 2019, he became the Science Director at the Canadian Light Source, Canada's synchrotron.

Website: https://www.bottonsgroup.com