

January Meeting

Machine Learning in Quantum Chemistry

Speaker: Jason Goodpaster, Assistant Professor of Chemistry and Chemical Physics, University of Minnesota Twin Cities

When: Wednesday, January 22nd
6:00pm - Social hour and dinner
7:00pm - Speaker

Where: Smith Hall, Room 117/119 for dinner and Room 331 for the speaker
207 Pleasant St SE, Minneapolis, 55455
The most convenient parking ramp is at the Weisman Art Museum (Smith Hall is within a short walking distance). Parking at the Weisman is \$3/hour. Go to campusmaps.umn.edu for an interactive campus map.

Menu: Buffet dinner provided by Holy Land Catering

Cost: \$15 / \$5 students; presentation only is free.
We prefer all payments using PayPal, however, we will accept payment at the door for those unable or unwilling. Please contact the treasurer, Shelby Auger (link to email address found on "Officers" link), prior to the event to let her know and we can plan accordingly.

RSVP: Please sign up by Monday, January 20th

Abstract: Machine Learning and data science is poised to revolutionize chemical research. As the field of machine learning has expanded, a variety of methodologies have become commonplace, such as kernel ridge regression, Gaussian process regression, and neural networks. In this talk, I will outline the basics of machine learning, the basics of these methodologies, and when these methodologies can and should be applied. Additionally, I will discuss the work my research group has been doing in applying these methodologies to quantum chemistry.

Bio: Jason Goodpaster is an assistant professor of chemistry and chemical physics at the University of Minnesota Twin Cities. His research focuses on the development of new quantum chemistry methods and applying these methods to a wide variety of chemical systems including: metal organic frameworks, inorganic catalysis, surface enhanced raman spectroscopy, and electrochemistry. Professor Goodpaster obtained his PhD at Caltech and performed his postdoctoral work at Lawrence Berkeley National Lab.