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Machine Learning for Molecular Properties and Chemistry

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Abstract

Computer simulation is foundational to modern theoretical chemistry. Calculating physical properties of molecular systems is paramount to drug development, bio-molecular simulation and materials design. These calculations must be fast and accurate to allow for high-throughput studies of small molecules or the simulation of large systems consisting thousands of atoms. Traditional methods for obtaining these properties are based on classical physics or quantum mechanical (QM) methods. Classical techniques are computationally efficient but have questionable accuracy when used outside their direct parametrization sets. QM based methods tend to be more accurate than their classical counterparts, however, their computational scaling is frequently prohibitively expensive to treat realistic systems. Machine learning-based (ML) QM property predictors are capable of fitting directly to QM data with low error while remaining computationally as fast as classical techniques. We present our work on developing and applying various models for QM property prediction, which are trained to large datasets. I will then show that they can be generalized well outside of the training set. The targeted properties include ground state potential energy and forces, various atomic charge schemes, dipoles and quadruples, infrared spectra, reduced Hamiltonians and a single model for singlet and triplet state energies and forces. Our results show the applicability of these accurate ML property predictors to systems many times larger than those in the training set with several magnitude speedup over reference QM methods, which is an exciting prospect for computational sciences.

Biography

Dr Sergei Tretiak received his MSc from the Moscow Institute of Physics and Technology and his PhD from the University of Rochester, where he worked with Professor Shaul Mukamel. He was then a Director-funded postdoctoral fellow at the Los Alamos National Laboratory (LANL) and became a LANL Staff Scientist in 2001. Since 2006, he is a Staff Scientist at the Center for Integrated Nanotechnologies (CINT). He serves as an Adjunct Professor at the University of California, Santa Barbara and at the Skolkovo Institute of Science and Technology. He became an APS Fellow (2014), LANL Fellow (2018), and received the LANL Postdoctoral Distinguished Mentor Award (2015) and the LANL Fellow's Prize for Research (2010). Dr Tretiak has supervised 23 postdoctoral fellows and mentored over 80 undergraduate and graduate students. He has published over 250 papers which have been cited over 13,000 times (H-index of 59, WoS) and has presented more than 250 invited and keynote talks.

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