New Horizons Solvay Lectures

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BIO: Alexandre Tkatchenko is a Professor of Theoretical Chemical Physics at the University of Luxembourg since 2015. He obtained his bachelor degree in Computer Science and a Ph.D. in Physical Chemistry at the Universidad Autonoma Metropolitana in Mexico City. In 2008–2010, he was an Alexander von Humboldt Fellow at the Fritz Haber Institute of the Max Planck Society in Berlin. Between 2011 and 2016, he led an independent research group at the same institute. Tkatchenko has given more than 190 invited talks, seminars and colloquia worldwide, published more than 120 articles in peer-reviewed academic journals (h-index=49), and serves on the editorial boards of Physical Review Letters and Science Advances (an open-access journal in the Science family). He received a number of awards, including the Gerhard Ertl Young Investigator Award of the German Physical Society, and two flagship grants from the European Research Council: a Starting Grant in 2011 and a Consolidator Grant in 2017. His group pushes the boundaries of quantum mechanics, statistical mechanics, and machine learning to develop efficient methods to enable accurate modeling and new insights into complex materials.

The Promise and Rise of Machine Learning in Chemistry and Physics

Learning from data has led to paradigm shifts in a multitude of disciplines, including web, text and image search, speech recognition, as well as bioinformatics. Can machine learning enable similar breakthroughs in understanding (quantum) molecules and materials? The main challenge is the disproportionately large size of chemical space, estimated to contain 10^60 molecules even when only counting small organic drug-like candidates. Aiming towards a unified machine learning (ML) model of quantum interactions, I will discuss the potential and challenges for using ML techniques in chemistry and physics. ML methods can not only accurately estimate molecular properties of large datasets, but they can also lead to new insights into chemical similarity, aromaticity, reactivity, and molecular dynamics. However, to do so one needs to carefully unify spatial and temporal physical symmetries with purpose-designed ML methods. While the potential of machine learning for revealing insights into complex quantum-chemical systems is high, many challenges remain. I will conclude my talk by discussing these challenges.

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