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Quantum-Chemical Insights from Deep Tensor Neural Networks[1]

KRISTOF T. SCHÜTT, FARHAD ARBABZADAH, STEFAN CHMIELA, KLAUS-ROBERT MÜLLER, Technische Universität Berlin, ALEXANDRE TKATCHENKO, University of Luxembourg — Discovery of novel materials can be guided by searching databases of known structures and properties. Indeed, electronic structure calculations and machine learning have recently been combined aiming towards the goal of accelerated discovery of chemicals with desired properties. However, the design of an appropriate descriptor is critical to the success of these approaches. Here we address this issue with deep neural tensor networks (DTNN): a deep learning approach that is able to learn efficient representations of molecules and materials [1]. The mathematical construction of the DTNN model provides statistically rigorous partitioning of extensive molecular properties into atomic contributions – a long-standing challenge for quantum-mechanical calculations of molecules. Beyond achieving accurate energy predictions (1 kcal mol^{-1}) throughout compositional and configurational space, DTNN provide spatially and chemically resolved insights into quantum-mechanical properties of molecular systems beyond those trivially contained in the training data. Thus, we propose DTNN as a versatile framework for understanding complex quantum-mechanical systems based on high-throughput electronic structure calculations. [1] K. T. Schütt et al., Nat. Comm. (2016).

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