# Machine Learning of Quantum Mechanical Operators using Deep Neural Networks: Achieving linear-scaling calculation of electron ionization by learning from low- dimensional tensors

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We present a general and computationally efficient method for machine learning of many- body quantum mechanical operators. The one particle Green's function, G (1,1') is the correlation function that is associated with the correlated many-electron wave function of chemical systems. The poles of the 1-particle Green's function contain information about ionization potentials (IPs) and electron-affinities (EAs) of many-electron systems. The goal of this work is to learn the Green's function using deep neural networks (DNN) and apply the DNN to calculate IPs of a series of semiconductor nanoparticles to assess their applicability in photovoltaic and light-harvesting applications.

One of the principle challenges in the construction of Green's functions is the unfavorable scaling of computational cost with respect to the increasing size of the chemical system. Specifically, the conventional method of constructing requires AO-to-MO transformation of integral ($N^5$ scaling), followed by the construction of 2-particle 1-hole and 1-particle 2-hole components of self-energy ($N^3$ scaling). Consequently, the conventional approach becomes computationally prohibitive for nanoparticles with 300+ heavy atoms with an excess of 5000 basis functions.

In this work, we address this computational bottleneck by machine-learning the Green's function operator using deep neural network. Specifically, we start with the frequency-domain representation of the one-particle Green's function and transform it into a real-space 13-dimensional kernel. We then show that the kernel can be factorized into tensor products of low-dimensional irreducible tensors. A series of DNNs are used to learn these low-dimensional tensors and which are then used in tandem to construct to full Green's function.

The main benefit of the present method is that it avoids the steep scaling associated with the traditional approach of constructing the Green's function. Specifically, we avoid AO-to-MO integral transformation and explicit representation of the operators in particle-hole basis. The principle computational cost comes from the training of the DNNs and numerical integration using Monte Carlo method, both of which do not exhibit the steep non-linear dependence on the number of molecular orbital basis functions. Consequently, this method can be applied to chemical system which are computationally impractical using conventional methods. The developed method was used for calculation of IP's in a series of PbS quantum dots (Pb4S4-P140S140) and the effect of the size of the quantum dots on IPs will be presented.