Środowe seminarium w Instytucie Fizyki

January 27th – 12:00

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"Solving the electronic Schrödinger equation with deep learning"

Variational quantum Monte Carlo provides a computationally efficient platform for arbitrarily accurate solutions of the electronic Schrödinger equation, but until recently the accuracy has been limited by the expressiveness of the available wave function ansatzes [1]. In this talk, I will present our deep-learning ansatz PauliNet [2], which takes advantage of deep neural networks as universal approximators to represent electronic wave functions with high fidelity. PauliNet uses a baseline HF solution and deep Jastrow factor and backflow transformation, and reaches state-of-the-art accuracy for systems ranging from diatomic molecules, to strongly correlated H_{10}, to cyclobutadiene (28 electrons).

[1] Foulkes, W. M. C., Mitas, L., Needs, R. J. & Rajagopal, G. Rev. Mod. Phys. 73, 33–83 (2001). `https://doi.org/10.1103/RevModPhys.73.33`
[2] Hermann, J., Schätzle, Z. & Noé, F. Nat. Chem. (2020). `https://doi.org/10.1038/s41557-020-0544-y`