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Abstract for an Invited Paper
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Quantum dynamics calculations enhanced by machine learning[1]

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I will describe how quantum dynamics calculations can benefit from Bayesian machine learning (ML). In particular, I will show that a hybrid approach, where ML is used to model the Hamiltonian parameters and parse the solutions of the Schrodinger equation, yields accurate quantum predictions with fewer calculations than traditional approaches; produces not only quantum observables but also the uncertainties of these observables stemming from limitations imposed by the difficulty of solving the Schrodinger equation; can be used to solve the inverse scattering problem; and can make accurate predictions of quantum observables for systems and experimental conditions that are currently out of reach of rigorous quantum theory. I will illustrate that it is possible to build Bayesian models that can extrapolate quantum solutions in the Hamiltonian parameter space. This can be used potentially to discover new physics of quantum systems at the Hamiltonian parameters, where neither theory nor experiment are feasible. Finally, I will illustrate that ML can be used to correct the results of approximate quantum dynamics calculations, offering a system- and approximation-independent approach to enhance the accuracy of quantum predictions. I will discuss how these methods can advance quantum theory of ultracold molecules. References: PCCP 21, 13392 (2019); PRL 121, 255702 (2018); PRL 115, 073202 (2015).

[1]NSERC of Canada