# Time-Domain Machine Learning approach for Extending the Timescales in Nonadiabatic Dynamics Simulations

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One of the key bottlenecks of atomistic nonadiabatic molecular dynamics (NA-MD) simulations is undoubtedly the underlying electronic structure calculations step, in which properties such as excited state energies and nonadiabatic couplings between states are obtained. As a result, modeling of slow quantum dynamical processes where long simulations are needed become increasingly difficult if not impossible, especially for nanoscale and periodic systems. To date, a number of approaches to extend the timescales of NA-MD calculations have been proposed, including those based on the use of cheaper electronic structure methods, machine learning (ML)-based potentials, as well as methods that directly extend the simulations by using ML-based predictors such as recurrent or short-long-term-memory networks, and so on.

As an alternative, I developed a ML-based approach for predicting the key properties needed for NA-MD propagation (energies or couplings) based simply on a single input parameter – time. The approach is based on using the auxiliary linearly-independent variables – modes – that are the explicit functions of time. The construction of this time-domain ML (TD-MD) approach will be discussed and its performance for model and atomistic systems will be discussed.

I will also briefly comment on the Kohn-Sham Hamiltonian mapping approach recently developed in our lab. The applications of this method to modeling nonradiative excitation energy relaxation as well as to NMR spin relaxation dynamics will be discussed.