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Emerging Research Fronts in Machine Learning for Studying Excited State Dynamics

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Deadline for manuscript submissions:
31 October 2024

Message from the Guest Editors

Dear Colleagues,

The study of excited-state dynamics is crucial for understanding phenomena such as photoabsorption, energy and charge transfers, photochemical reactions, etc. Traditional computational methods for studying excited-state dynamics face significant challenges in terms of computational cost and accuracy; thus, they are often limited to small systems with short dynamics. The emergence of machine learning is revolutionizing computational chemistry and materials science, providing novel methods to address these challenges in modeling excited-state dynamics.

This Special Issue aims to cover recent advances in the development and application of machine learning in studying excited-state dynamics. The topic of interest include, but are not limited to, methods and/or applications in the following areas:

- Excited-state machine learning force fields;
- Excited-state property prediction with machine learning;
- Solar cell design with machine learning;
- Nonadiabatic excited-state dynamics with machine learning;
- Machine learning exciton dynamics;
- Machine learning for quantum dynamics.

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Message from the Editor-in-Chief

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