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Machine Learning Interactions for Chemical Reactions: Validation and Applications

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In this talk I will describe neural network and kernel-based methods suitable to construct full-dimensional, reactive potential energy surfaces for molecular dynamics studies. The focus will be on validating the PESs and using them for computing observables to compare with experiments. An additional aspect concerns the role of numerical accuracy and uncertainty quantification which emerge as an important technical aspect. Illustrative examples ranging from triatomics to molecules relevant to atmospheric chemistry will be discussed.