Abstract Submitted
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Machine learning for molecular scattering dynamics: Gaussian Process models for improved predictions of molecular collision observables[1] ROMAN KREMS, JIE CUI, ZHIYING LI, University of British Columbia — We show how statistical learning techniques based on kriging (Gaussian Process regression) can be used for improving the predictions of classical and/or quantum scattering theory. In particular, we show how Gaussian Process models can be used for: (i) efficient non-parametric fitting of multi-dimensional potential energy surfaces without the need to fit ab initio data with analytical functions; (ii) obtaining scattering observables as functions of individual PES parameters; (iii) using classical trajectories to interpolate quantum results; (iv) extrapolation of scattering observables from one molecule to another; (v) obtaining scattering observables with error bars reflecting the inherent inaccuracy of the underlying potential energy surfaces. We argue that the application of Gaussian Process models to quantum scattering calculations may potentially elevate the theoretical predictions to the same level of certainty as the experimental measurements and can be used to identify the role of individual atoms in determining the outcome of collisions of complex molecules. We will show examples and discuss the applications of Gaussian Process models to improving the predictions of scattering theory relevant for the cold molecules research field. More details: PRL 115, 073202 (2015).

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