

Machine learning prediction of a chemical reaction over 8 decades of energy

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Recent progress in machine learning has sparked increased interest in utilizing this technology to predict the outcomes of chemical reactions. The ultimate aim of such endeavors is to develop a universal model that can predict products for any chemical reaction given reactants and physical conditions. In pursuit of ever more universal chemical predictors, machine learning models for atom-diatom and diatom-diatom reactions have been developed, yet no such models exist for termolecular reactions. Accordingly, we introduce neural networks trained to predict opacity functions of atom recombination reactions. Our models predict the recombination of $\text{Sr}^+ + \text{Cs} + \text{Cs} \rightarrow \text{SrCs}^+ + \text{Cs}$ and $\text{Sr}^+ + \text{Cs} + \text{Cs} \rightarrow \text{Cs}_2 + \text{Sr}^+$ over multiple orders of magnitude of energy, yielding overall results with a relative error $\lesssim 10\%$. Even far beyond the range of energies seen during training, our models predict the atom recombination reaction rate accurately. As a result, the machine is capable of learning the physics behind the atom recombination reaction dynamics.

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Machine learning (ML), within the context of artificial intelligence, is transforming the current paradigm in the physical sciences, ushering in the big data era. In this emerging paradigm, the methodology involves using data directly to identify patterns and predict the behavior of complex systems. In this regard, the calculation of the outcome of a chemical reaction is one of the most demanding and needed tasks in modern chemical physics. As a result, considerable effort has been dedicated to using data-driven approaches in chemical physics to predict chemical reactions [1–6]. For instance, several methods have been developed to accelerate the calculation of multidimensional potential energy surfaces [7–13], the essential element for reaction dynamics calculations. Similarly, the prediction of reaction barrier heights—the bottleneck to understanding many essential chemical reactions—is recently gaining more attention [14–20]. In the case of complex chemical reactions, machine learning is used to automate reaction networks in intricate chemical scenarios [21–25].

Despite significant progress, the main goal remains elusive: a universal chemical predictor. A universal predictor would take a set of reactants and physical properties (like temperature and density) and predict the products of the reaction and their branching ratios. It has been possible to predict the outcome of atom-diatom and diatom-diatom reactions [26–33] for a given set of reactants or across the isotopologue space [34]. The next level of complexity is the study of higher-order reactions, specifically termolecular reactions (i.e., third-order

chemical reactions involving the mutual interaction between three reactants). Termolecular reactions play a crucial role in a multitude of fundamental physicochemical processes spanning more than 14 orders of magnitude in energy from plasma physics to ultracold atoms [35–37]. One of the most well-studied and relevant termolecular reactions is atom recombination, in which two atoms form a bound state while the third one carries away the excess kinetic energy [38–42]. Even more interesting is the ion-atom-atom recombination reaction, which results in the formation of either a molecular ion or a molecule, depending on the collision energy [43,44]. However, despite its relevance, no effort has been made to apply ML techniques to the prediction of these reactions.

In this Letter, using a feedforward neural network (FNN) approach, we predict probabilities for ion-atom-atom recombination in an energy range between 10^{-4} and 10^4 K with a $\lesssim 5\%$ relative error, ranging from cold chemistry to plasma physics applications. The machine is capable of learning the reaction properties coming from long-range and short-range physics. Furthermore, it excellently predicts the maximum impact parameter for the reaction to occur—the essential element for the calculation of the reaction rate. The reaction rates are calculated from the ML-predicted reaction probabilities, yielding excellent agreement in both the low and high collision energy regimes. Moreover, the ML model can correctly extrapolate the reaction rates for collision energies well beyond the range explored in the training set, demonstrating that the machine can learn the reaction dynamics of atom recombination reactions.

To train any ML model to predict probabilities for atom recombination reactions, we must first obtain a detailed and representative training dataset. Here, the training dataset is obtained using the classical trajectory calculation method in hyperspherical coordinates, which has been shown to yield accurate results versus experimental data for a wide range of collision energies [43–46]. Since the methodology has been

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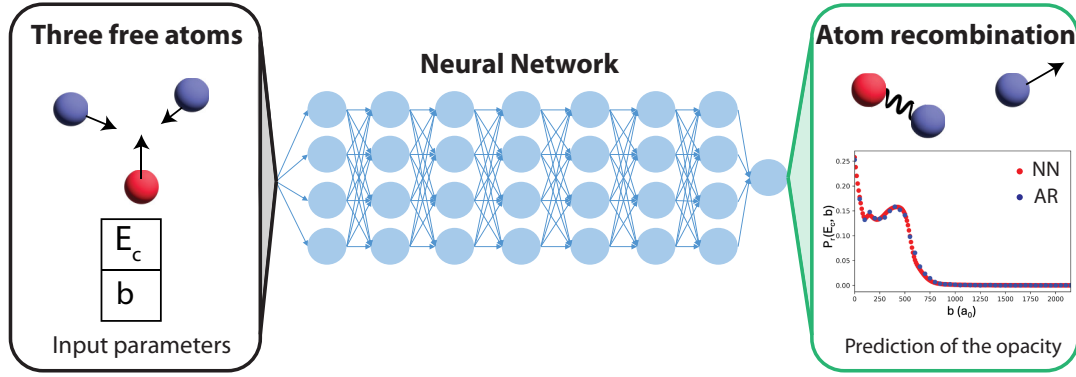


FIG. 1. Displayed above is the overall scheme of this work. The collision energy E_c and impact parameter b are the model features, and the opacity function $P_r(E_c, b)$, which determines the probability of reaction, is the model target. The models developed in this work are meant to predict opacities for molecular formation resulting from the mutual collision of three atoms. The neural network shown here exactly depicts the architecture (layers and neurons) of the neural network models used in this work.

previously introduced, we discuss it only briefly here [37]. The main idea is to map the three-body problem of three interacting particles of masses m_i and positions $\mathbf{r}_i$, $i = 1, 2, 3$, into a single-particle problem in a six-dimensional (6D) space. The three-body Hamiltonian is given by

$$H = \frac{\mathbf{p}_1^2}{2m_1} + \frac{\mathbf{p}_2^2}{2m_2} + \frac{\mathbf{p}_3^2}{2m_3} + V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), \quad (1)$$

and after neglecting the trivial center of mass motion, the Hamiltonian reads

$$H = \frac{\mathbf{p}_{6D}^2}{2\mu} + V(\rho_{6D}), \quad (2)$$

where $\mu = \sqrt{\frac{m_1 m_2 m_3}{m_1 + m_2 + m_3}}$ is the reduced three-body mass, ρ_{6D} is the position in 6D configuration space, and $\mathbf{p}_{6D}$ is the conjugate momentum. In this space, it is straightforward to calculate the recombination cross section, resembling the standard two-body classical scattering cross section expression and given by

$$\sigma_r(E_c) = \frac{8\pi^2}{3} \int_0^{b_{\max}(E_c)} P_r(E_c, b) b^4 db, \quad (3)$$

where E_c is the collision energy, b is the impact parameter, $b_{\max}$ is the maximum impact parameter for which recombination occurs at a given E_c , and $P_r(E_c, b)$ is the so-called opacity function or reaction probability, representing the probability of a particular reaction as a function of E_c and b . For a given E_c and b , we run n_{tot} trajectories and the products of the collision are tracked for each trajectory, yielding n_r trajectories resulting in a reaction; hence,

$$P_r(E_c, b) = \frac{n_r}{n_{\text{tot}}} \pm \frac{\sqrt{n_r}}{n_{\text{tot}}} \sqrt{\frac{n_{\text{tot}} - n_r}{n_{\text{tot}}}}, \quad (4)$$

where the uncertainty is a statistical result arising from the Monte Carlo sampling technique taking into account that the reaction probability is a Boolean function. Finally, the energy-dependent atom recombination rate can be found by considering the volume (in 6D) of product formed per unit

time

$$k_3(E_c) = \sqrt{\frac{2E_c}{\mu}} \sigma_r(E_c). \quad (5)$$

The reactants of choice are $\text{Sr}^+ + \text{Cs} + \text{Cs}$, whose reaction present two possible products: the molecular ion reaction channel $\text{Sr}^+ + \text{Cs} + \text{Cs} \rightarrow \text{SrCs}^+ + \text{Cs}$ and the molecule reaction channel $\text{Sr}^+ + \text{Cs} + \text{Cs} \rightarrow \text{Sr}^+ + \text{Cs}_2$. Interestingly enough, all ion-atom-atom reactions present the same physics, and hence a single reaction is enough to check the viability of the machine learning approach to the cited reactions [47]. We calculate the opacities for both reaction products in a range of energies between 10^{-4} and 10^4 K. We use a feedforward neural network to predict the opacity function as a function of E_c and b . This was done because once all of the individual trajectories are summed over at fixed E_c and b , the probability of reaction becomes a function of solely E_c and b [see Eq. (4)]. Indeed, to calculate the energy-dependent cross sections and reaction rates, we need the opacity function as a function of E_c and b [see Eqs. (3) and (5)]. The FNN architecture used in this work [see Fig. 1] is fully connected, which means the outputs of each neuron in a given layer are fed into every neuron in the following layer. The models were trained on the opacity functions generated from classical trajectory simulations. The features for the models were the collision energy E_c and the impact parameter b . However, since some of the reaction probabilities can be very small, it proved better to learn $\sqrt{P_r(E_c, b)}$. Two models were trained, one for SrCs^+ formation and another for Cs_2 formation, and both had the same architecture, namely the one depicted in Fig. 1. The model for SrCs^+ formation is referred to as NN-ion and the remaining model NN-mol. The models each have 137 tunable parameters (weights plus biases). The activation function used for all neurons except the lone neuron in the final layer was the softplus activation function. The final layer's neuron uses the sigmoid activation function, which ensures the outputs, meant to be (the square root of) probabilities, are in $[0, 1]$.

The training dataset is generated from classical trajectories, using Lennard-Jones potentials assuming pairwise interactions, which has been shown to be an excellent approximation

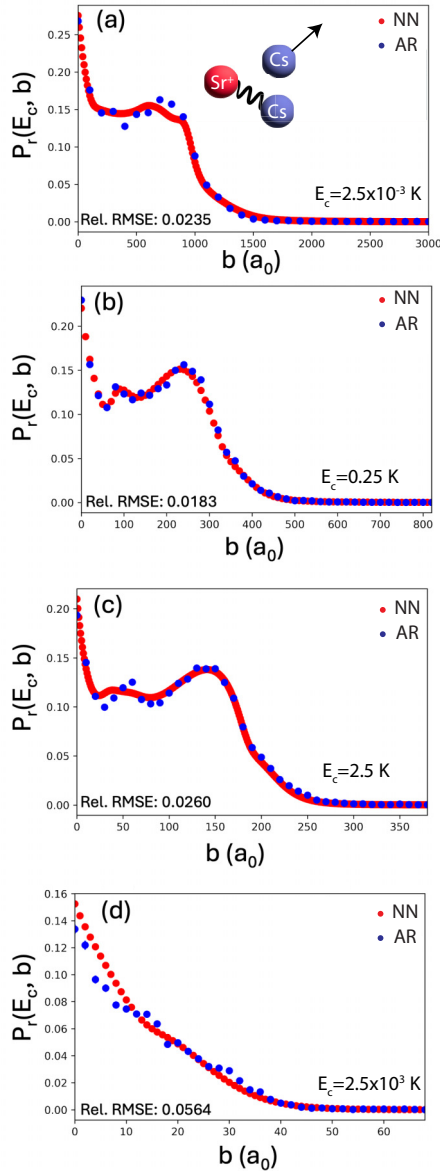


FIG. 2. FNN prediction of opacity functions for the formation of SrCs^+ . Data points in red represent neural network predictions, and those in blue represent the results generated from classical trajectories (AR for atom recombination). Given also are the relative RMSE between predictions and simulation results.

[48]. The parameters for the potentials (in atomic units) are $C_6 = 6.64 \times 10^3$ and $C_{12} = 6.63 \times 10^8$ for Cs-Cs, and $C_4 = 200$ and $C_8 = 1.67 \times 10^6$ for Cs- Sr^+ [49–51]. The classical trajectories were calculated using the software package PY3BR [52]. For NN-ion, the energies used for training are $E_c \in [0.1 \text{ mK}, 1 \text{ mK}, 10 \text{ mK}, 0.1 \text{ K}, 1 \text{ K}, 10 \text{ K}, 100 \text{ K}, 1000 \text{ K}, 5000 \text{ K}, 10000 \text{ K}]$, and we run 10^4 trajectories per impact parameter at all E_c . For NN-mol, the training energies are $E_c \in [10 \text{ K}, 100 \text{ K}, 1000 \text{ K}, 10000 \text{ K}]$, but 5×10^4 trajectories per impact parameter are required due to its typically small reaction probability. For all opacities in the training (or test) datasets, it was ensured that the maximum impact parameter b_{max} was reached (or exceeded)

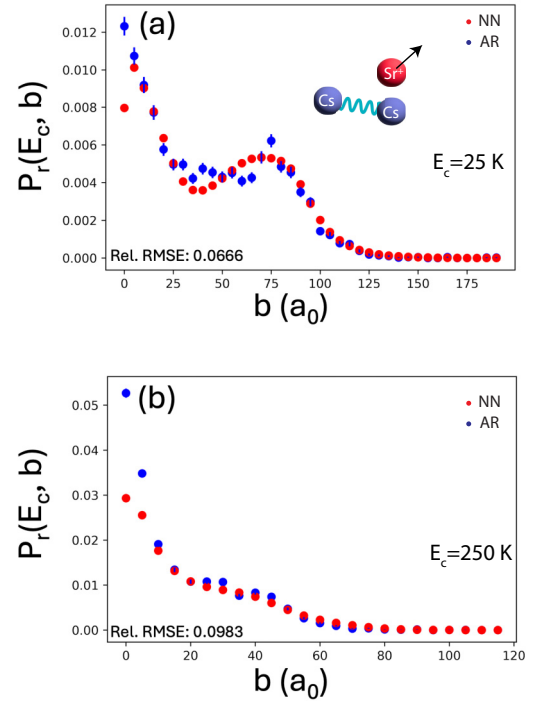


FIG. 3. FNN prediction of opacity functions for the formation of Cs_2 . Data points in red represent neural network predictions, and those in blue represent the results generated from classical trajectories (AR for atom recombination) including the error bars at one standard deviation as prescribed by Eq. (4). Given also are the relative RMSE between predictions and simulation results.

by inspecting each opacity. For training, the Adam optimizer was used to fit the models' parameters with a learning rate of 0.007 [53]. Glorot normal initialization was used to initialize the parameter values [54]. The mean squared error loss function was used. NN-ion was trained using $\sim 20\,000$ epochs to a final loss of $\sim 10^{-4}$, and NN-mol was trained using 10 000 epochs to a final loss of $\sim 1.3 \times 10^{-5}$. The FNNs were designed and trained using the TensorFlow package and Keras API [55].

The results showcasing the ability of the NN-ion model developed in this work are shown in Fig. 2. Each panel represents a different value of E_c and shows the variation of the reaction probability with b . All of the values of E_c used for the test results in Fig. 2 are within the range of E_c used for the model's training dataset. Also provided are the relative root-mean-squared error (RMSE) values comparing the NN predictions to the results from classical trajectory simulations (denoted by "AR"). It is clear from Fig. 2 that NN-ion demonstrates excellent predictive power over a wide range of energies. Indeed, NN-ion was trained on 8 decades of E_c , and Fig. 2 confirms that NN-ion makes accurate predictions throughout that energy range. All of the relative RMSE values in Fig. 2 are below 6%, and NN-ion captures the opacity function throughout the entire range $b \in [0, b_{\text{max}}]$. Furthermore, it is clear, especially from panel (b), that NN-ion can predict the details of the variation of the opacity for intermediate values of b , although we notice a systematic deviation at high collision energies, as shown in panel (d). Most importantly,

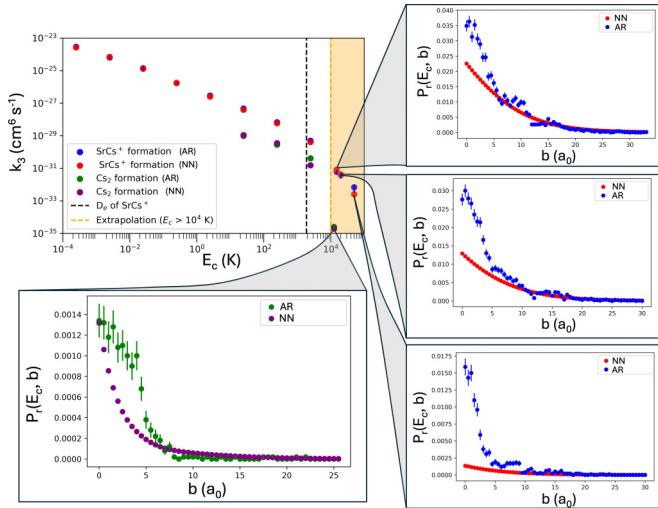


FIG. 4. Energy-dependent atom recombination reaction rates k_3 , for both SrCs^+ and Cs_2 formation for the collision energies used in the test datasets. In the k_3 plot, red points indicate SrCs^+ formation rates calculated from NN predicted opacities, and those in blue indicate the rates calculated from classical trajectory simulations (AR for atom recombination) including the error bars at one standard deviation as prescribed by Eq. (4). Also, Cs_2 formation is represented by purple points for those rates calculated from NN predicted opacities, and green points represent those rates calculated from classical trajectory simulations. The black dashed line indicates where the threshold law takes effect, which corresponds to the dissociation energy of SrCs^+ ($D_e \approx 1888$ K [52]). The orange-shaded region indicates the extrapolation regime where the models predict opacities for collision energies greater than any included in the training dataset.

the NN captures the change of the opacity function from the low-energy regime to the high-energy regime around the dissociation energy of the molecular ion. In other words, the machine is able to differentiate short-range from long-range dominated atom recombination reactions, depending on the collision energy. Moreover, the NN is capable of locating b_{max} for every collision energy.

Representative results for NN-mol are given in Fig. 3, and as in Fig. 2, every panel stands for the opacity as a function of the impact parameter for a given collision energy. Specifically, panel (a) corresponds to an E_c of 25 K and panel (b) corresponds to an E_c of 250 K. This model shows a relative RMSE of 10%, coming mostly from the intermediate to small values of the impact parameters. However, as we show below, these errors will have little impact on the atom recombination rate since large impact parameters contribute the most. Thus, we may also note that for molecular formation, the model successfully learns the long-range behavior of the opacity function and anticipates b_{max} , two properties of the model that are essential for effective rate prediction. It is clear that the NN approach to predicting opacity functions is universal between the reaction channels of an atom recombination reaction provided that separate models, having the same architecture, are trained on the different channels.

Here, we go beyond the interpolating regime by asking the machine for predictions in a totally unseen range of energies, very different from the ones the machine has been exposed

too. Most machine learning methods have a difficult time with this task. Energy-dependent atom recombination reaction rates were calculated from both the classical trajectory simulations and the corresponding NN predictions for the test dataset, and the results are shown in Fig. 4, where the main panel shows the energy-dependent atom recombination rates as a function of the collision energy. At low collision energies, the reaction rate follows a power law until reaching the binding energy of the molecular ion (black dashed line) where a new trend emerges. This change of trend is due to the role of the short-range region of the atom-ion interaction potential, establishing the onset of high-energy collisions where the molecular formation channel starts to be comparable to molecular ion production. Therefore, for collision energies larger than the threshold, the predictions should be more involved due to the role of both short-range and long-range effects on the reaction dynamics. As displayed in Fig. 4, the NN-ion and NN-mol models are able to capture the regions of the opacity function having medium to large values of the impact parameter. As a result, the energy-dependent predicted reaction rates agree extremely well with the calculations.

Our work shows that machine learning techniques for the prediction of chemical reactions are readily applicable to high-order reaction rates such as atom recombination reactions. We show that machine learning models, specifically feedforward neural networks, can efficiently learn atom recombination reactions in a collision energy range spanning from 10^{-4} to 10^4 K, or equivalently, between 8.62×10^{-9} and 8.62×10^{-1} eV. We are able to predict the opacities for molecular ion recombination and molecule formation, showing the potential of machine learning techniques for termolecular reactions. Furthermore, the machine learning approach offers a substantial computational speedup: The opacity function for a given E_c can be predicted by an NN in 60–130 ms, whereas the classical trajectory approach could take 1–4 h. Using ML-predicted opacities, it is possible to calculate atom recombination cross sections and energy-dependent reaction rates. More spectacular is the fact that, even in the extrapolation regime where the collision energy is well beyond the greatest energy of the training dataset, both models perform extremely well, yielding very accurate reaction rates. The predicted reaction rates are accurate even when the model struggles to accurately capture the short impact parameter region. Alternatively, the machine is capable of differentiating short-range from long-range effects as a function of the collision energy, showing that the machine learns the physics behind the opacity function. It is worth noting that despite the strength of our models, there are conceivable ways to make our approach more universal. Namely, a single model could be developed that predicts both the ion and molecule formation channels simultaneously. Our results open up a new avenue for machine learning techniques in the physical sciences: termolecular reactions.

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Data availability. The data that support the findings of this Letter are openly available [56], embargo periods may apply.

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