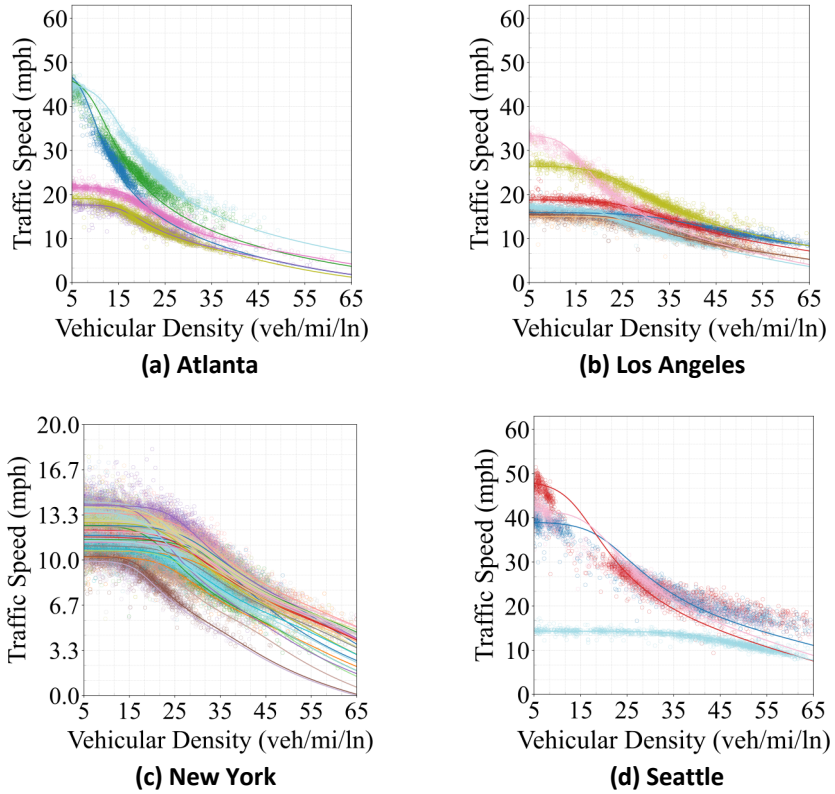
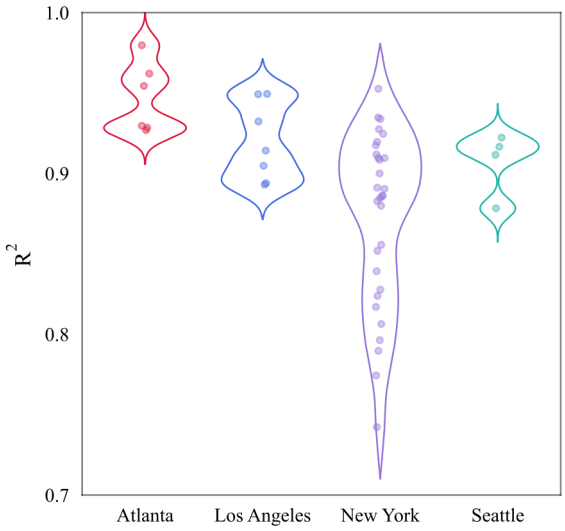
Supplementary Information

Supplementary Note 1: Macroscopic Traffic Model

The relationship between traffic volume and speed in urban networks can be estimated at the subregional scale using the concept of the network Macroscopic Fundamental Diagram (MFD) [36-40]. The MFD provides an analytical framework for efficient yet accurate modeling of macroscopic traffic by estimating the relationships between network traffic variables using aggregated traffic data [41-47]. In this research, we adopt the MFD concept to estimate the relationship between traffic speed and vehicular density and accordingly derive the speed-volume relationship at the subregional level in downtown Atlanta, Los Angeles, New York, and Seattle. The estimated speed-volume relationship is then used to predict traffic speed under projected increases in traffic volume. To this end, we train a log-sum-exp regression model [48] to estimate the macroscopic speed-density relationship for each subregion, as plotted in **Supplementary Figure 1a**. The training data include traffic speed and vehicular density aggregated over 15-minute time intervals at the subregional scale using a data-fusion approach [49]. **Supplementary Figure 1b** presents the distribution of R^2 values for the estimated speed-density relationships in downtown Atlanta, Los Angeles, New York, and Seattle.



(a) Estimated Speed-Density Relationships at the Subregional Level. The color of each scatter series and its corresponding fitted curve represents the associated subregion, consistent with the color coding used in Figure 1.



(b) Distribution of R^2 Values for the estimated Speed-Density Relationships at the Subregional Level

Supplementary Figure 1. Estimated Relationships between Traffic Speed and Vehicular Density, with Corresponding 95% Confidence Intervals, at the Subregional Level Across Atlanta, Los Angeles, New York, and Seattle. Traffic data are aggregated over 15-minute intervals for each subregion and preprocessed using a quantile-based approach. Across all four cities, traffic speed decreases as vehicular density increases, reflecting the progressive deterioration of traffic with increasing congestion. Atlanta and Seattle exhibit comparatively high free-flow speeds and pronounced speed reductions as density increases, whereas New York shows consistently lower speeds and greater variation among subregions. Los Angeles has a more gradual and relatively consistent decline in speed across its subregions. The R^2 distributions indicate that the estimated speed-density relationships generally achieve a high goodness of fit, with Atlanta showing the highest and most concentrated values, while New York has the widest variation in model performance across subregions.

Supplementary Note 2: Vehicle Energy Consumption and Emissions Model

Vehicle fuel consumption and the resulting emissions largely depend on vehicle type, fuel, and age. Given the traffic volumes and compositions (i.e., the breakdown of traffic volume by vehicle type, fuel, and age) based on the registration data, a deep learning model is developed to estimate vehicle fuel consumption and emission rates per vehicle mile traveled based on vehicle type, fuel, and age at varying traffic speeds. The model is trained on EPA MOVES4 simulation results for Atlanta, Los Angeles, New York, and Seattle to estimate fuel consumption rates and emission rates of CO_2, NO_x, and PM2.5 from tires and brakes, in addition to EV electricity consumption, at varying speeds from 2.5 to 75 mph based on three vehicle attributes: (1) type (combination long-haul truck, combination short-haul truck, light commercial truck, motorhome [recreational vehicle], motorcycle, other buses, passenger truck, passenger car, refuse truck, school bus, single-unit long-haul truck, single-unit short-haul truck, and transit bus), (2) fuel (compressed natural gas [CNG], diesel fuel, electricity, ethanol [E-85], and gasoline), and (3) age (0 to 30 years).

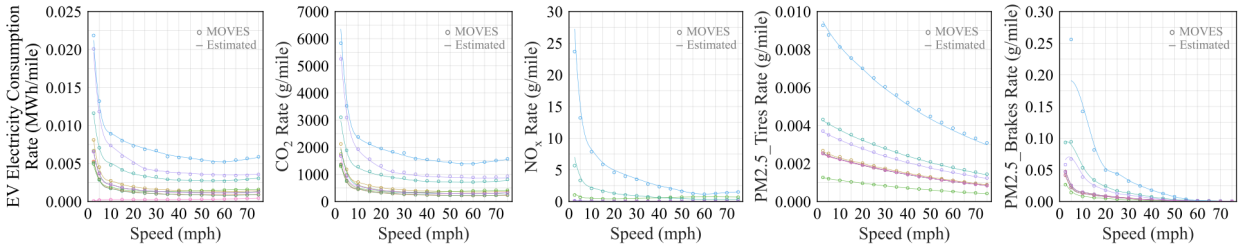
The training data consist of fuel consumption and emission rates, as well as EV electricity consumption rates, at various speeds for all existing combinations of vehicle type, fuel, and age in the state vehicle registration database. In preparing the training data, we encode the categorical variables of the model, i.e., vehicle type and fuel, using the one-hot encoding approach. We also apply the Yeo-Johnson (YJ) transformation to improve the normality and homoscedasticity of the data [50]. To train the proposed

feedforward neural network model, we use backpropagation with the Adaptive Moment Estimation (ADAM) algorithm [51] and a learning rate of 0.001 to optimize the model parameters. Training this deep learning model using the MOVES4 inventory eliminates the need for numerous simulation runs, which can be time-consuming and computationally expensive, to estimate the energy consumption and emissions of heterogeneous vehicles in mixed traffic based on vehicle type, fuel, and age at varying traffic speeds. **Supplementary Table 1** summarizes the performance metrics of our deep learning model compared with MOVES simulation results in predicting energy consumption, including fuel and electricity consumption, and emission rates in Atlanta, Los Angeles, New York, and Seattle.

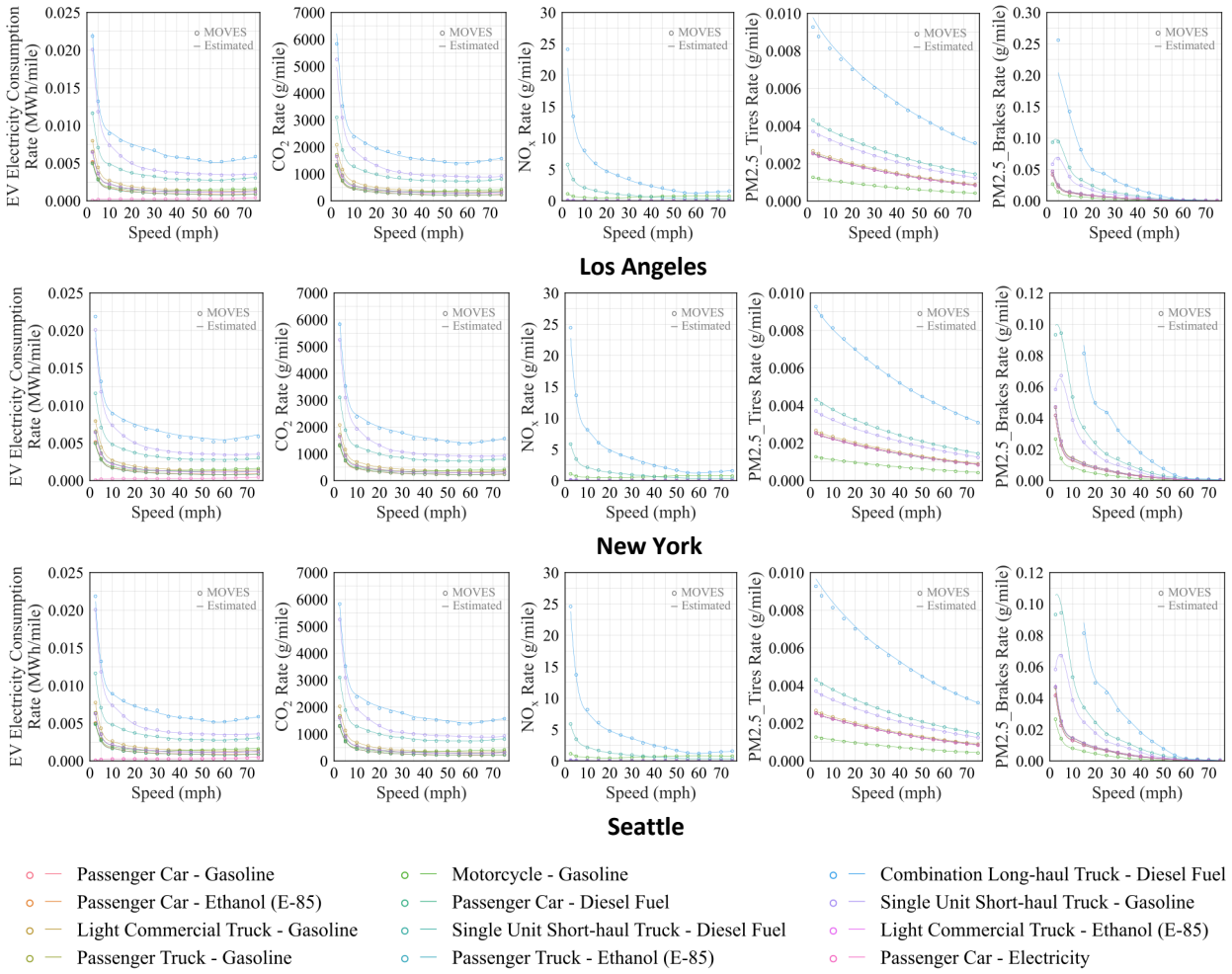
Supplementary Table 1. Performance Metrics of the Deep Learning Emissions Model Compared with MOVES Simulations for Predicting Energy Consumption, Including Fuel and Electricity Consumption, and Emission Rates. The low values of RMSE, MAE, and MAPE and the high R^2 values indicate the strong performance of the deep learning model in predicting energy consumption and emission rates in Atlanta, Los Angeles, New York, and Seattle.

	Feed-Forward Neural Network Performance Metrics																			
	Fuel/Electricity Consumption				CO_2				NO_x				PM2.5_Brakes				PM2.5_Tires			
City	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE	R^2
Atlanta	0.054	0.030	0.252	0.997	0.063	0.040	0.260	0.996	0.039	0.025	0.083	0.999	0.064	0.025	0.168	0.996	0.051	0.023	0.277	0.997
Los Angeles	0.044	0.026	0.213	0.998	0.067	0.044	0.333	0.996	0.038	0.025	0.096	0.999	0.045	0.017	0.067	0.998	0.042	0.017	2.586	0.998
New York	0.064	0.038	0.335	0.996	0.048	0.029	0.168	0.998	0.030	0.020	0.086	0.999	0.060	0.025	0.180	0.996	0.055	0.025	0.373	0.997
Seattle	0.045	0.027	0.206	0.998	0.038	0.025	0.126	0.999	0.023	0.017	0.096	1.000	0.051	0.023	0.084	0.997	0.038	0.018	2.034	0.999

Supplementary Figure 2 plots the simulated and estimated rates of energy consumption and emissions of CO_2, NO_x, and PM2.5 from tires and brakes for a selected subset of 2024 vehicles (gasoline passenger car, E-85 passenger car, gasoline light commercial truck, gasoline passenger truck, gasoline motorcycle, diesel passenger car, diesel short-haul truck, E-85 passenger truck, diesel long-haul truck, gasoline short-haul truck, E-85 commercial truck, and electric passenger car) at varying traffic speeds in Atlanta, Los Angeles, New York, and Seattle. Interestingly, vehicle energy consumption and air pollutant emission rates vary slightly with humidity, temperature, altitude, and other exogenous factors across different locations. The effects of these exogenous factors on energy consumption and air pollutant emission rates, which vary by vehicle type, fuel, and age, are captured in the simulation data used for model training. After successful training, our deep learning model provides continuous and accurate estimates of vehicle fuel consumption and air pollutant emission rates, as well as EV electricity consumption, at varying traffic speeds for all vehicle classes based on their type, fuel, and age. Note that the energy consumption and emission rates of CO_2 and NO_x per vehicle mile traveled are minimized at an optimal speed that varies by vehicle type, fuel, age, and location.



Atlanta



Supplementary Figure 2. Estimated and Simulated EV Electricity Consumption and Vehicle Emission Rates for 2024 Model-Year Vehicles at Varying Traffic Speeds in Atlanta, Los Angeles, New York, and Seattle. The deep learning model provides continuous estimates of energy consumption and emission rates without requiring numerous MOVES runs, which can be time-consuming and computationally intensive. Although the overall patterns are similar across the four cities, slight differences in emission rates arise from variations in humidity, temperature, altitude, and other location-specific factors incorporated into the simulation data used for model training. In general, vehicle energy consumption and the emission rates of CO_2 and NO_x per vehicle mile traveled decrease as traffic speed increases to an optimal level and then begin to increase with further increases in speed.

Our deep learning model also enables continuous and accurate estimation of EV electricity consumption, as well as vehicle fuel consumption and emission rates, based on vehicle type, fuel, and age at varying traffic speeds in different locations. The high accuracy and efficiency of this deep learning approach enable bypassing the limiting need for numerous simulation runs, which can often be time-consuming and computationally intensive.

Supplementary Note 3: EV Charging Emissions Model

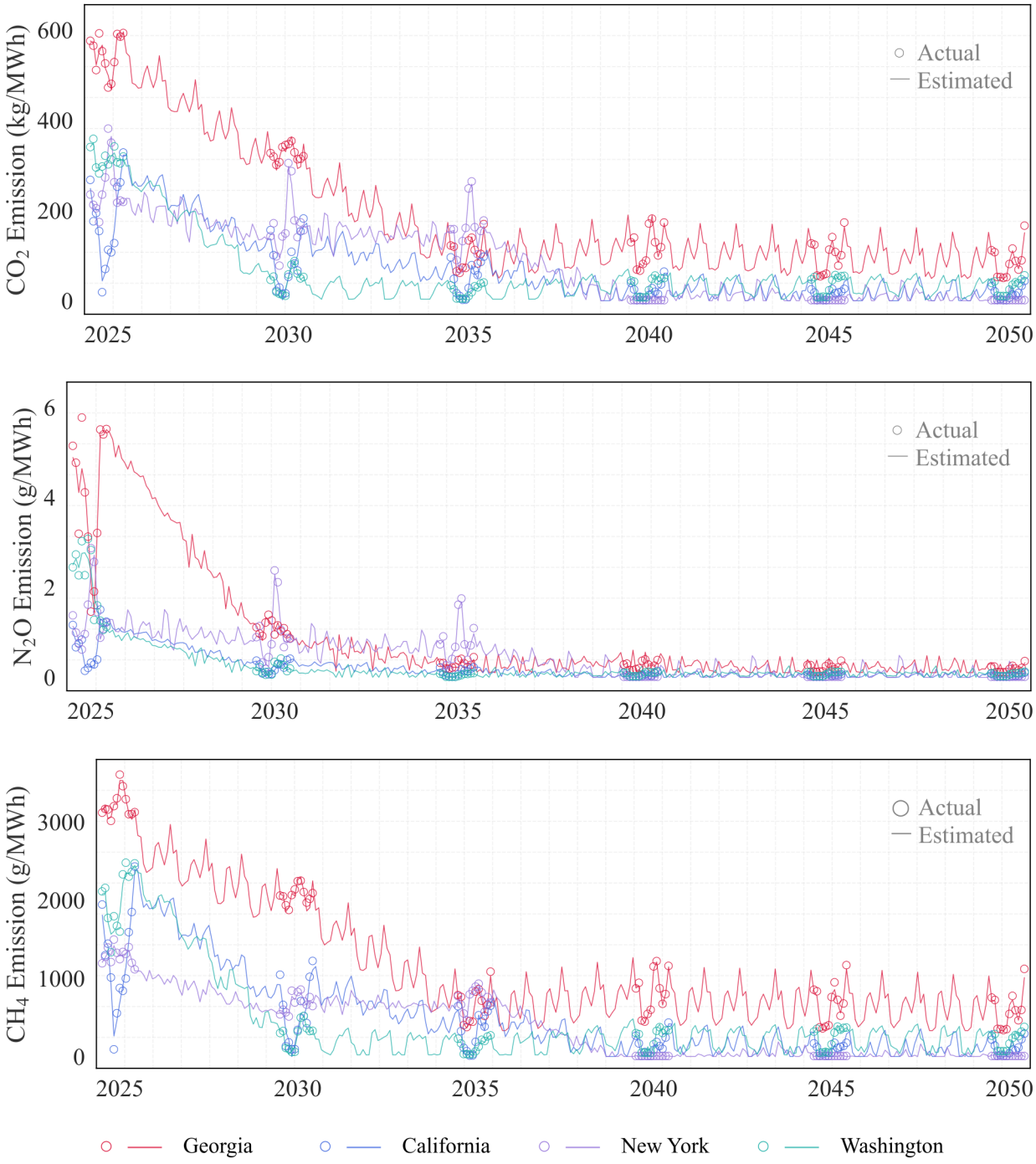
Electricity consumption by EVs for battery charging increases upstream emissions from the power grid, which depend directly on power generation technologies, distribution network efficiency, temporal load distribution, and the electricity generation mix across different energy-sector regions. To capture upstream emissions from EV charging, we develop a machine learning model on the Prophet platform [53] and train it on simulation data from Cambium, developed by NREL [52]. Prophet, developed by Meta, is a flexible and robust time-series forecasting platform [53] that is well suited to data exhibiting strong temporal patterns, seasonal effects, missing observations, and outliers. To enable predictive analysis of grid emissions resulting from EV charging, the Prophet model is trained on Cambium simulation results. Cambium projects the evolution of power generation and distribution systems and provides a comprehensive framework for simulating electric-sector operations across the United States. After successful training, this machine learning model enables accurate and continuous predictions of carbon dioxide (CO_2), nitrous oxide (N_2O), and methane (CH_4) emissions resulting from EV charging over future months and years through 2050. **Supplementary Table 2** summarizes the performance metrics of our machine learning model compared with Cambium simulations under the mid-case scenario [35, 52] for Georgia, California, New York, and Washington.

Supplementary Table 2. Performance Metrics of Our Machine Learning Model Compared with Cambium Simulation Results for Predicting Emission Rates per MWh of EV Electricity Consumption for Battery Charging Under the Mid-case Scenario. The low values of RMSE, MAE, and MAPE and the high R^2 values indicate the high accuracy of our machine learning model in predicting upstream EV charging emission rates per MWh of additional electricity consumption in Georgia, California, New York, and Washington.

State	EV Charging Emission Model											
	CO_2				N_2O				CH_4			
	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE	R^2
Georgia	36.85	29.36	19.20	0.95	0.30	0.23	24.67	0.96	166.47	113.91	11.42	0.96
California	11.91	9.30	74.21	0.98	0.08	0.06	37.27	0.92	69.96	53.60	118.19	0.98
New York	14.73	9.00	5.98	0.98	0.17	0.11	15.94	0.95	54.14	33.79	4.30	0.99
Washington	11.51	9.51	45.94	0.95	0.08	0.05	32.42	0.98	72.42	58.67	54.07	0.92

The proposed machine learning framework captures both long-term temporal trends and seasonal variations in simulated grid-emission rates at a monthly resolution, avoiding reliance on simple interpolation between widely separated projection years. Cambium provides emissions projections for all 12 months of each five-year benchmark (2025, 2030, 2035, 2040, 2045, and 2050) but does not provide monthly values for the intervening years. This temporal structure limits its direct use in continuous, high-resolution analyses because grid emission rate can vary substantially from month to month while electricity demand evolves continuously over time. By training the Prophet model on the monthly simulation outputs available for the benchmark years, the proposed approach learns the underlying seasonal and long-term patterns and generates continuous monthly projections that remain consistent with Cambium outputs while filling the temporal gaps between benchmark years. Once trained, the model provides accurate and continuous predictions of CO_2, N_2O, and CH_4 emission rates through 2050 (the additional emissions from power plants associated with a 1 MWh increase in electricity consumption for EV charging). By avoiding the need for repeated complex simulations, the proposed machine learning

model facilitates efficient prediction of EV charging emissions under different projections of technology costs, fuel prices, demand growth, and electricity-sector policies. **Supplementary Figure 3** plots the learned monthly patterns of CO_2, N_2O, and CH_4 emission rates from EV charging from 2025 to 2050 under the mid-case scenario.



Supplementary Figure 3. Learned Monthly Patterns of EV Charging Emission Rates from 2025 to 2050 Under the Mid-case Scenario. CO_2 emission rates generally decline substantially across all four states, although the timing and magnitude of the reductions vary. Washington has the most rapid decline and approaches near-zero emission rates

around 2030, reflecting its cleaner electricity mix, while California also shows a pronounced reduction. New York declines more gradually and reaches near-zero levels around 2040. Georgia experiences a substantial reduction but maintains the highest CO_2 emission rates throughout the projection period because of its continued reliance on fossil-fuel generation. After approximately 2035, emission rates generally stabilize at relatively low levels while continuing to have monthly fluctuations. N_2O emission rates follow a similar declining pattern. Washington and California approach near-zero levels relatively early, while New York reaches near-zero levels around 2040. Georgia shows the largest absolute reduction but continues to exhibit higher N_2O emission rates than the other states through 2050. CH_4 emission rates also decline markedly, with Washington showing the fastest initial reduction, followed by California. New York declines more gradually before approaching near-zero levels around 2040, whereas Georgia retains the highest CH_4 emission rates despite a substantial overall decrease. The recurring fluctuations in the predicted series reflect the monthly and seasonal variation captured by the machine learning model.