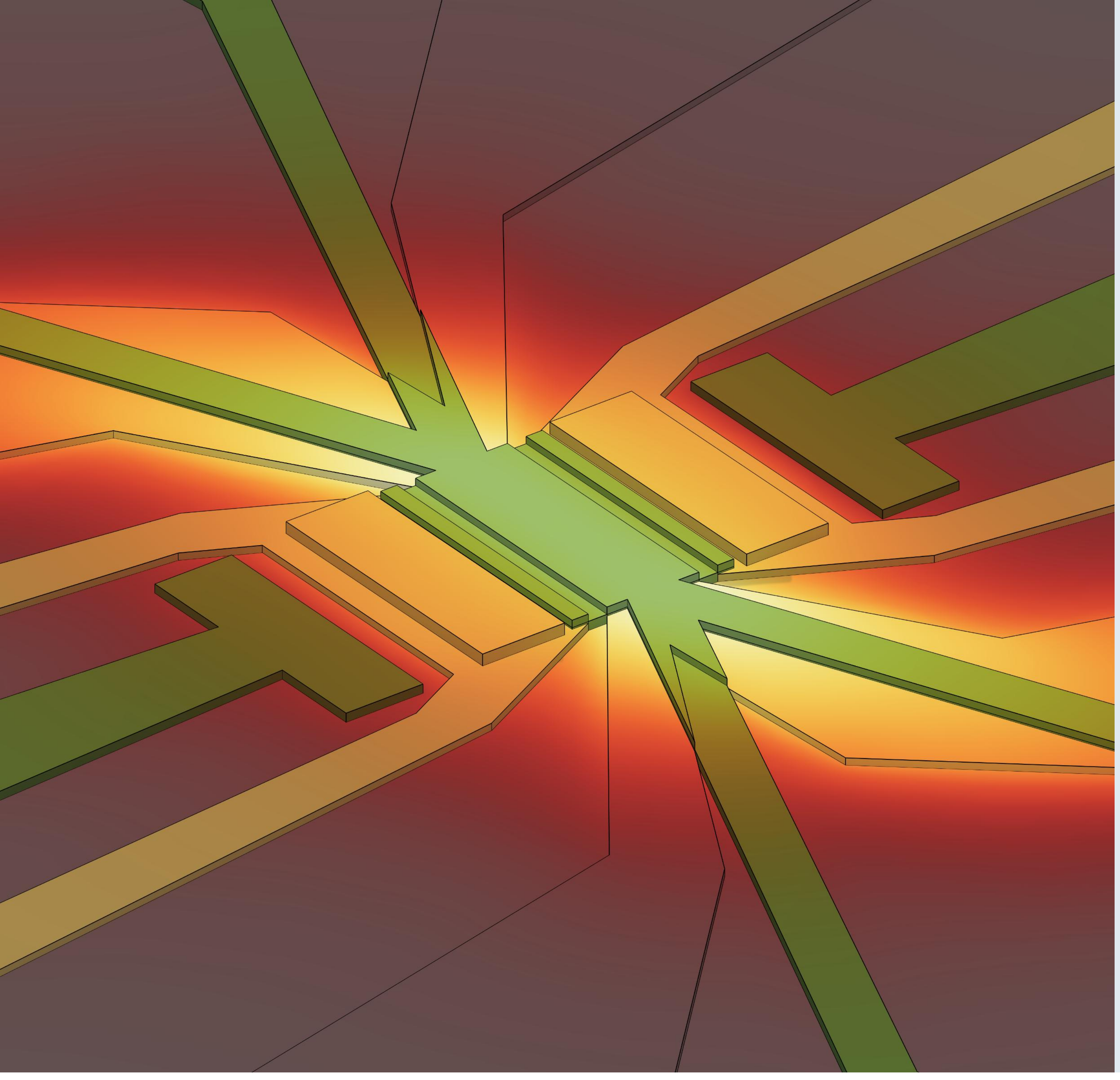

Thermoelectric Simulation in a Quantum Heat Engine Device

The performance of a quantum heat engine depends on its thermal and electrostatic environment. This work details the design optimization of embedded micro-heater, heat dissipation, and gate coupling for a quantum dot heat engine device.

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Abstract

Quantum heat engines (QHEs) perform a thermodynamic cycle by exchanging heat between a hot and a cold reservoir employing quantum systems as the working medium. Such thermoelectric generators could theoretically reach Curzon-Ahlborn efficiency due to the excellent properties of the quantum dots (QDs) as energy filters [1]. We use finite element modeling in COMSOL Multiphysics® to simulate the key components of the device. An electro-thermal model of Joule heating from an applied AC current is used to analyze the resulting temperature gradient (ΔT), which is crucial to quantify the maximum Seebeck effect that can be extracted from the real device. Separately, an electrostatic model determines the gate coupling parameter for controlling the GNR's quantum energy levels, which depends on the device geometry and the oxide material. The results provide critical design parameters that inform the device fabrication strategy and the interpretation of experimental transport measurements.

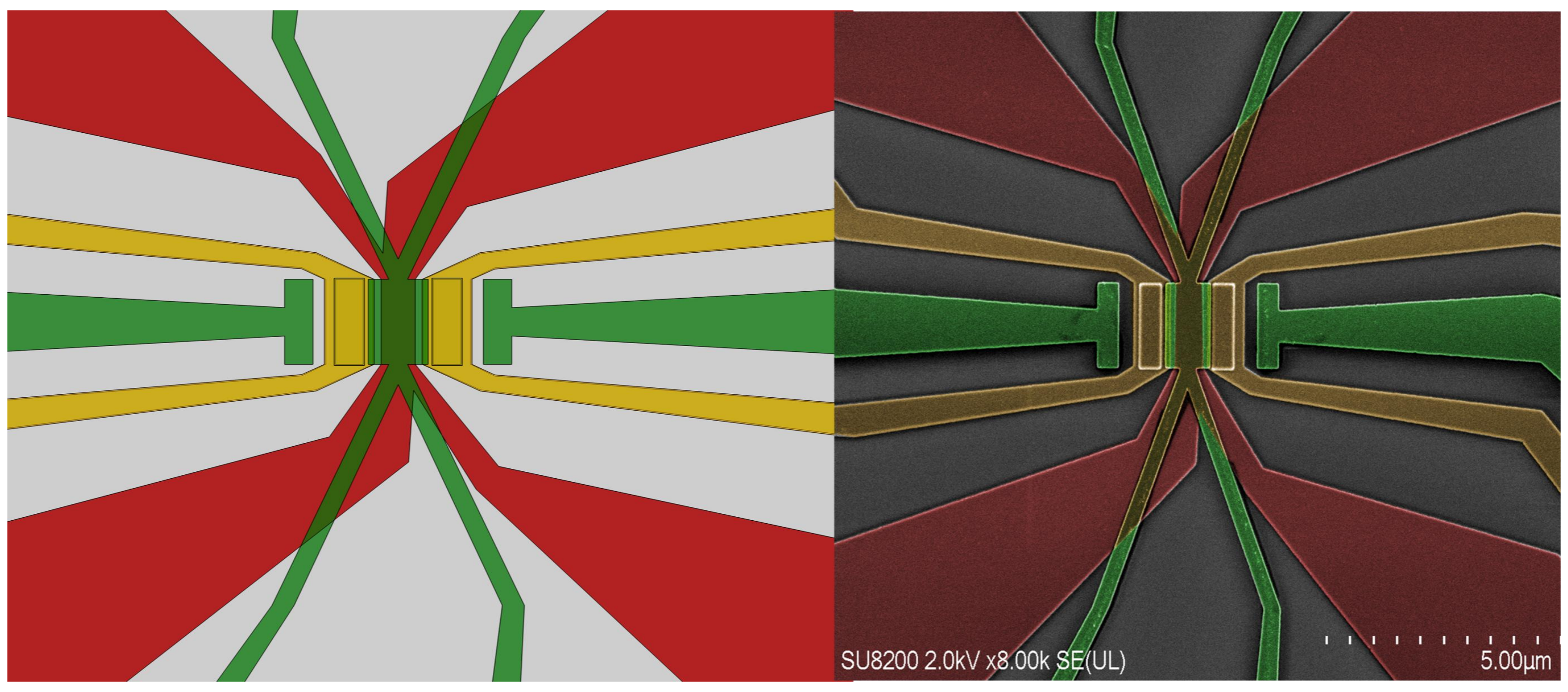

Figure 1. *Left:* COMSOL® model of the quantum dot heat engine, showing the device geometry. *Right:* False-colored SEM image of the fabricated device, highlighting the same structural sections as in the model for direct comparison.

Methodology

Electro-Thermal Simulation: The *Electric Currents* and *Heat Transfer in Solids* modules were coupled using the *Joule Heating* multiphysics node. A time-dependent study was performed by applying a 3 Hz AC current to the microheater. The external faces of the substrate were fixed to room temperature to act as a thermal sink.

Electrostatic Simulation: The *Electric Currents* module was used to simulate the electrostatic effect of the gate electrodes. A 1V potential was applied to the gate terminal. The needle-like structures, which model the metallic source/drain electrodes in the final device, were included to accurately account for their electrostatic screening effect on the nanogap.

Results

The electro-thermal model reveals the device's frequency-dependent thermal response. At a low input frequency of 3 Hz, the temperature oscillates at 6 Hz (2ω), a key signature of Joule heating ($P \propto I^2$) that enables experimental lock-in detection [2]. At high frequencies (1 MHz), the heater's thermal inertia prevents it from fully cooling between cycles, causing a DC increase in its base temperature.

The electrostatic simulation calculates the potential profile in the nanogap (Fig. 2, bottom right). From this, we extract the gate coupling parameter, which quantifies the influence of the gate voltage on the GNR's energy levels after accounting for electrostatic screening from the source and drain electrodes.

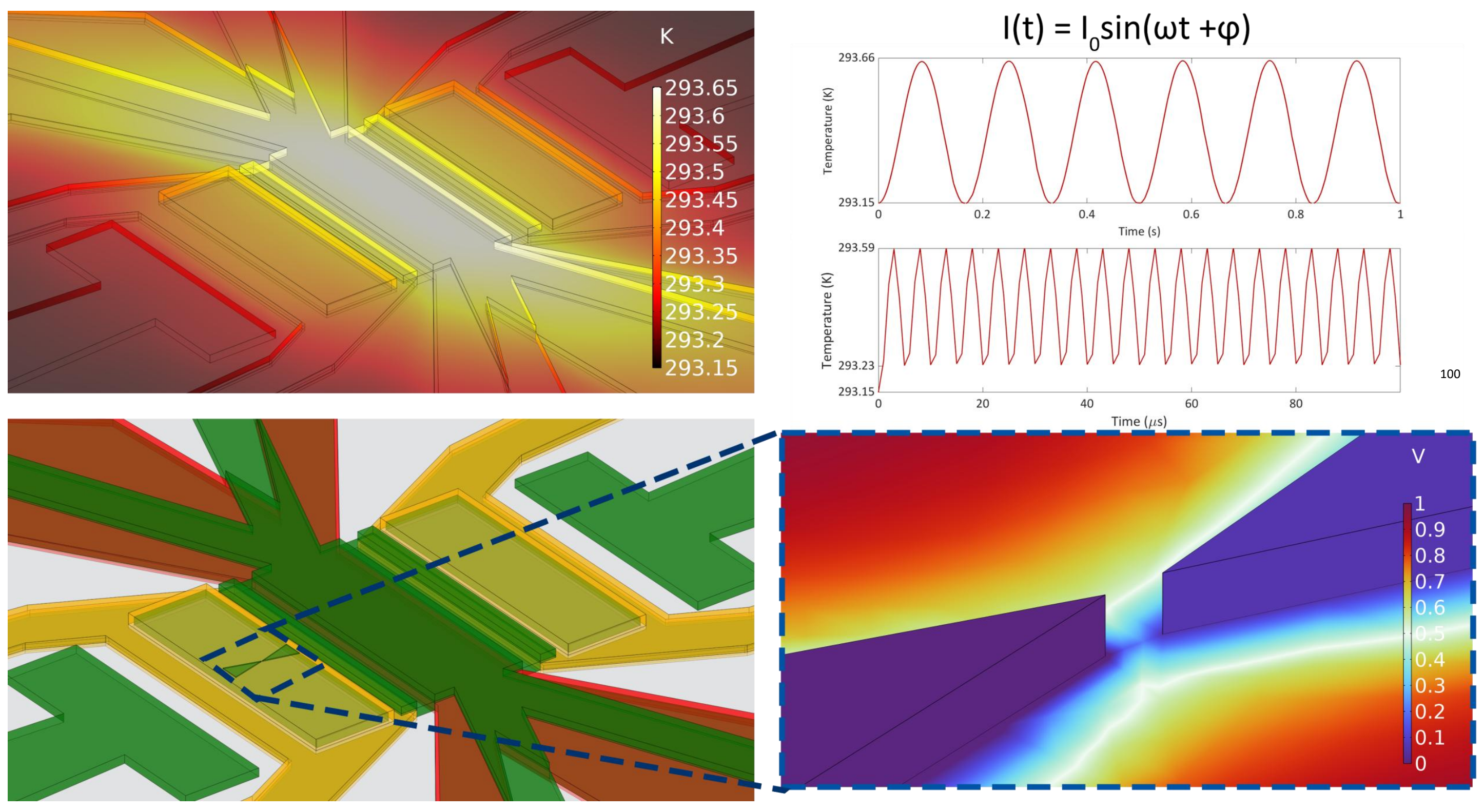

Figure 2. *Top left:* Simulated temperature profile at the peak amplitude of the applied AC current. *Top right:* Time evolution of the maximum temperature reached at 3Hz and 1MHz. *Bottom left:* Device with needle-shaped contacts used for electrical measurements. *Bottom right:* Zoom-in of the simulated electric potential distribution.

REFERENCES

[1] Josefsson, M., Svilans, A., Burke, A.M. et al., A quantum-dot heat engine operating close to the thermodynamic efficiency limits. Nature Nanotech 13, 920–924 (2018).

[2] Gehring, P., Sowa, J.K., Hsu, C. et al., Complete mapping of the thermoelectric properties of a single molecule. Nat. Nanotechnol. 16, 426–430 (2021).

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