

Thermal electromagnetic transport mediated by coupled surface phonon-polaritons in nanostructures

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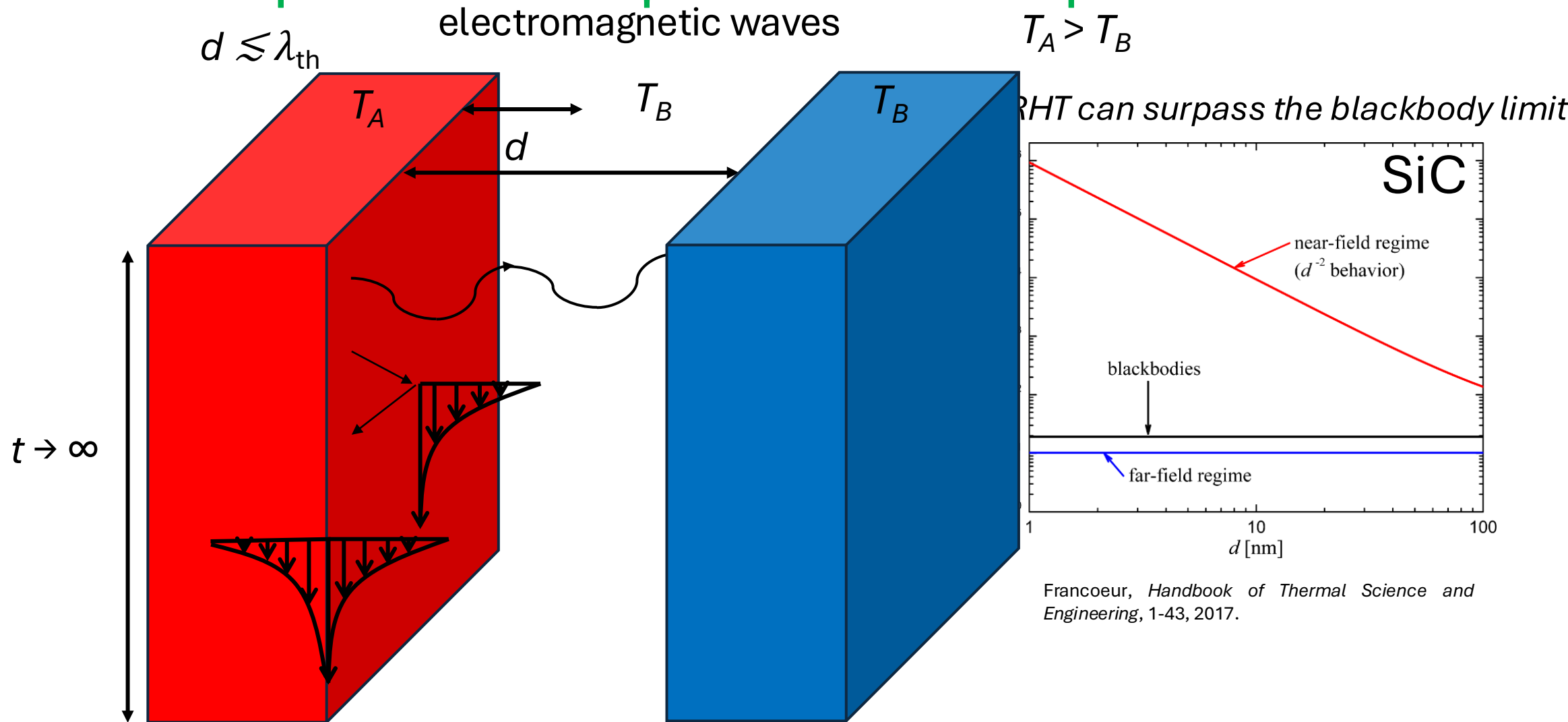
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Performance Computing

Near-field radiative heat transfer



When present, SPPs become the dominant type of mode contributing to NFRHT

Near-field radiative heat transfer is calculated via fluctuational electrodynamics

- Maxwell's equations (Rytov et al., *Principles of statistics radiophysics*, Springer-Verlag, 1989):

$$\nabla \times \mathbf{E}(\mathbf{r}, \omega) = i\omega\mu_0\mathbf{H}(\mathbf{r}, \omega)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, \omega) = -i\omega\varepsilon(\mathbf{r}, \omega)\varepsilon_0\mathbf{E}(\mathbf{r}, \omega) + \mathbf{J}^{(\text{fl})}(\mathbf{r}, \omega)$$

Fluctuating thermal current source

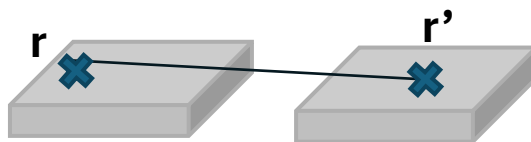
- Fluctuation-dissipation theorem:

$$\langle \mathbf{J}^{(\text{fl})}(\mathbf{r}, \omega) \mathbf{J}^{(\text{fl})\dagger}(\mathbf{r}', \omega') \rangle = 4\pi\omega \text{Im}[\varepsilon(\mathbf{r}, \omega)] \Theta(\omega, T) \delta(\mathbf{r} - \mathbf{r}') \delta(\omega - \omega') \bar{\mathbf{I}} \text{ where } \Theta(\omega, T) = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

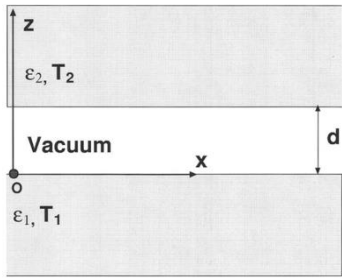
- Electric field is defined using the volume integral technique:

$$\mathbf{E}(\mathbf{r}, \omega) = i\omega\mu_0 \int_{V_{\text{therm}}} \bar{\mathbf{G}}(\mathbf{r}, \mathbf{r}', \omega) \mathbf{J}^{(\text{fl})}(\mathbf{r}', \omega) d^3\mathbf{r}', \quad \mathbf{r} \in \mathbb{R}^3$$

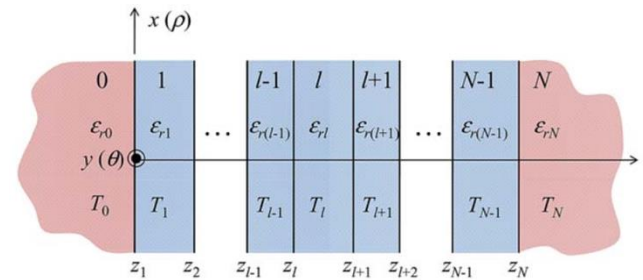
System Green's function



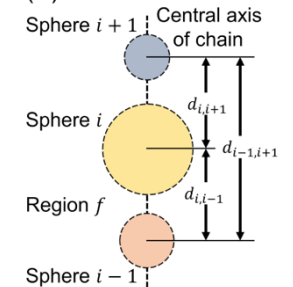
Most near-field radiative heat transfer (NFRHT) problems are solved analytically



Mulet et al., *Microscale Thermophys. Eng.* **6**, 209-222, 2002.

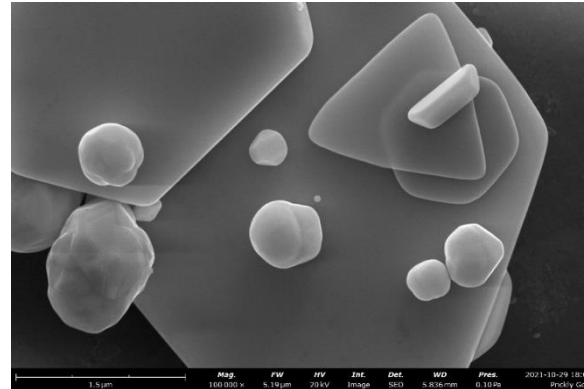


Francoeur et al., *JQSRT* **110**, 2002-2018, 2009.



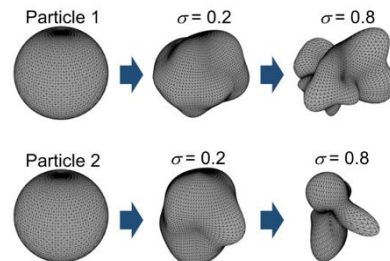
Czapla and Narayanaswamy, *JQSRT* **227**, 4-11, 2019.

Analytical solutions become intractable for complex geometries

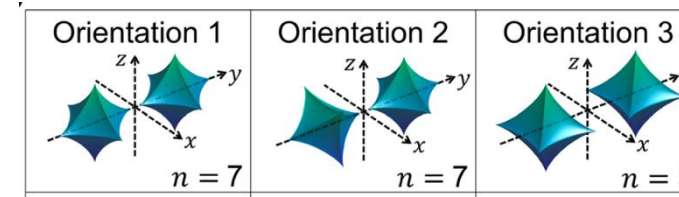


<https://www.nanoscience.com/techniques/scanning-electron-microscopy/>

We developed a numerical methodology based on FE for NFRHT between complex-shaped objects called the discrete system Green's function (DSGF)



Walter et al., *Physical Review B* **106**, 195417, 2022.



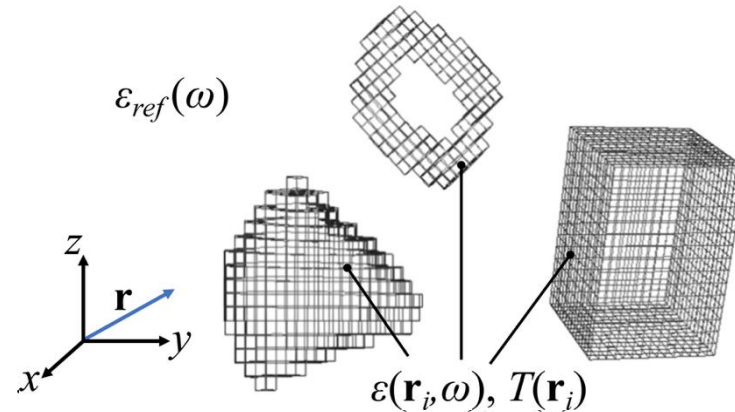
Walter and Francoeur, *Applied Physics Letters* **121**, 182206, 2022.

The DSGF solver computes numerically SGF from a linear system of equations

- The system Green's function (SGF) equation:

$$\bar{\bar{\mathbf{G}}}^0(\mathbf{r}, \mathbf{r}', \omega) = \bar{\bar{\mathbf{G}}}(\mathbf{r}, \mathbf{r}', \omega) - k_0^2 \int_{V_{\text{therm}}} \bar{\bar{\mathbf{G}}}^0(\mathbf{r}, \mathbf{r}'', \omega) \varepsilon_r(\mathbf{r}'', \omega) \bar{\bar{\mathbf{G}}}(\mathbf{r}'', \mathbf{r}', \omega) d^3 \mathbf{r}''$$

- The thermal sources are discretized into cubical subvolumes:



Walter et al., *Phys. Rev. B* **106**, 195417, 2022.

Walter et al., *Light, Plasmonics and Particles*, Chapter 11, 2023.

Corrêa et al., *JQSRT* **328**, 109163, 2024.

<https://github.com/Discrete-System-Greens-Function>

$$\left\{ \begin{bmatrix} \bar{\mathbf{I}} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \bar{\mathbf{I}} \end{bmatrix} - k_0^2 \begin{bmatrix} \bar{\bar{\mathbf{G}}}_{11}^0 & \cdots & \bar{\bar{\mathbf{G}}}_{1N}^0 \\ \vdots & \ddots & \vdots \\ \bar{\bar{\mathbf{G}}}_{N1}^0 & \cdots & \bar{\bar{\mathbf{G}}}_{NN}^0 \end{bmatrix} \begin{bmatrix} \alpha_1^{(0)} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \alpha_N^{(0)} \end{bmatrix} \right\} \begin{bmatrix} \bar{\bar{\mathbf{G}}}_{11} & \cdots & \bar{\bar{\mathbf{G}}}_{1N} \\ \vdots & \ddots & \vdots \\ \bar{\bar{\mathbf{G}}}_{N1} & \cdots & \bar{\bar{\mathbf{G}}}_{NN} \end{bmatrix} = \begin{bmatrix} \bar{\bar{\mathbf{G}}}_{11}^0 & \cdots & \bar{\bar{\mathbf{G}}}_{1N}^0 \\ \vdots & \ddots & \vdots \\ \bar{\bar{\mathbf{G}}}_{N1}^0 & \cdots & \bar{\bar{\mathbf{G}}}_{NN}^0 \end{bmatrix} \text{ where } \boxed{\bar{\bar{\mathbf{G}}}_{ij}} = \begin{bmatrix} G_{xx} & G_{xy} & G_{xz} \\ G_{yx} & G_{yy} & G_{yz} \\ G_{zx} & G_{zy} & G_{zz} \end{bmatrix}$$

$$\alpha_i^{(0)} = \Delta V_i \varepsilon_r(\mathbf{r}_i, \omega)$$

or simply as

$$\bar{\mathbf{A}} \bar{\mathbf{G}} = \bar{\bar{\mathbf{G}}}^0$$

9N² terms to be calculated

The Green's functions are directly applied to compute thermal quantities of interest

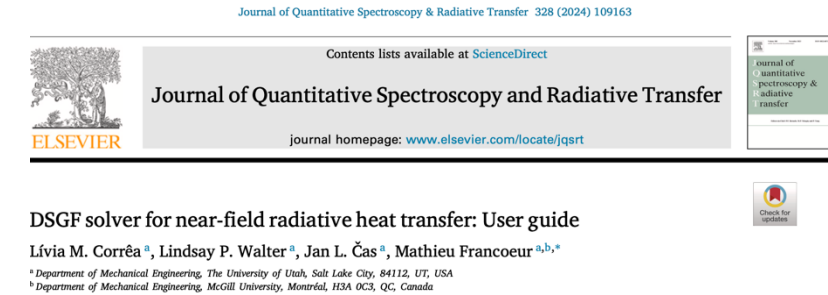
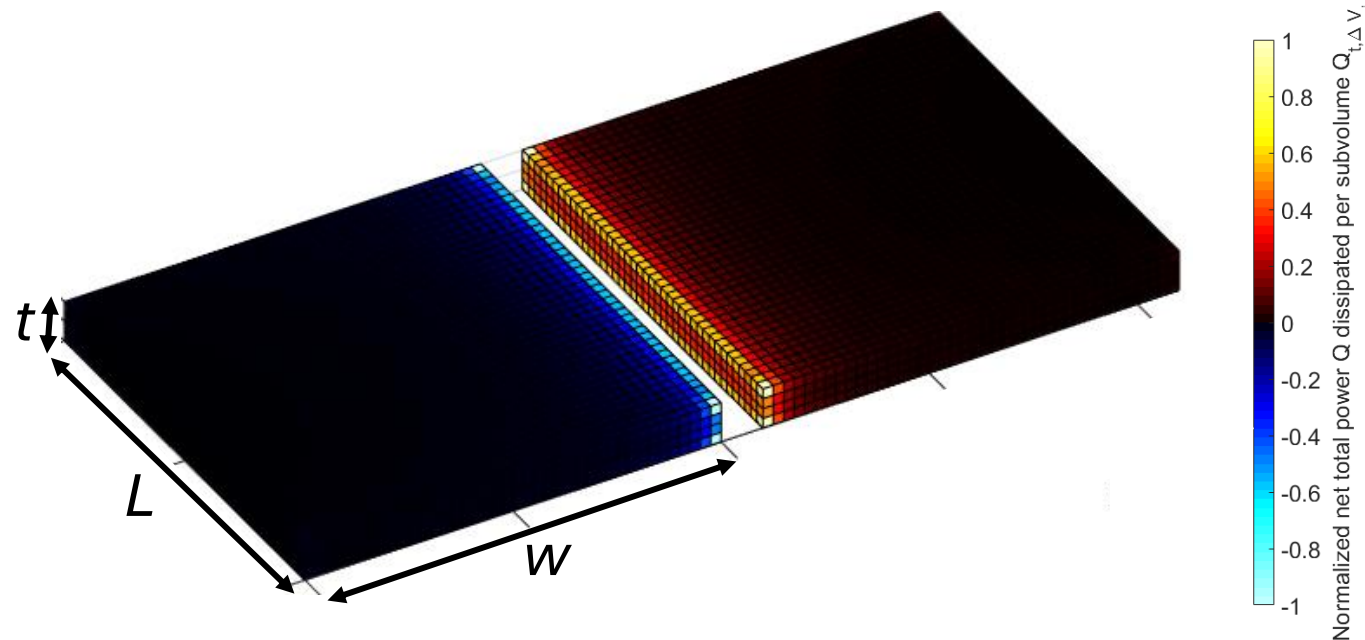
- Power dissipated between subvolumes:

$$\langle Q_{\Delta V_i}(t) \rangle = \frac{1}{2\pi} \int_0^\infty \left\{ \sum_{\substack{j=1 \\ j \neq i}}^N [\Theta(\omega, T_j) - \Theta(\omega, T_i)] \tau_{ij}(\omega) \right\} d\omega,$$

- where $\tau_{ij}(\omega)$ is the transmission coefficient:

$$\tau_{ij}(\omega) = 4k_0^4 \Delta V_i \Delta V_j \text{Im}[\varepsilon(\mathbf{r}_i, \omega)] \text{Im}[\varepsilon(\mathbf{r}_j, \omega)] \text{Tr}[\bar{\bar{\mathbf{G}}}(\mathbf{r}_i, \mathbf{r}_j, \omega) \bar{\bar{\mathbf{G}}}^\dagger(\mathbf{r}_i, \mathbf{r}_j, \omega)]$$

Multiscale simulation between SiC membranes, $t = 100$ nm,
 $w = 1 \mu\text{m}$, and $L = 1 \mu\text{m}$

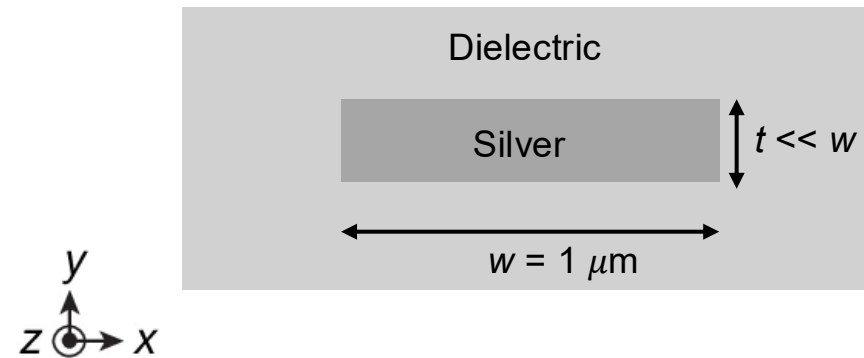


Corrêa et al., *JQSRT* **328**, 109163, 2024.

<https://github.com/Discrete-System-Greens-Function>



Motivation: How does EM corner and edge modes impact radiative heat transfer?

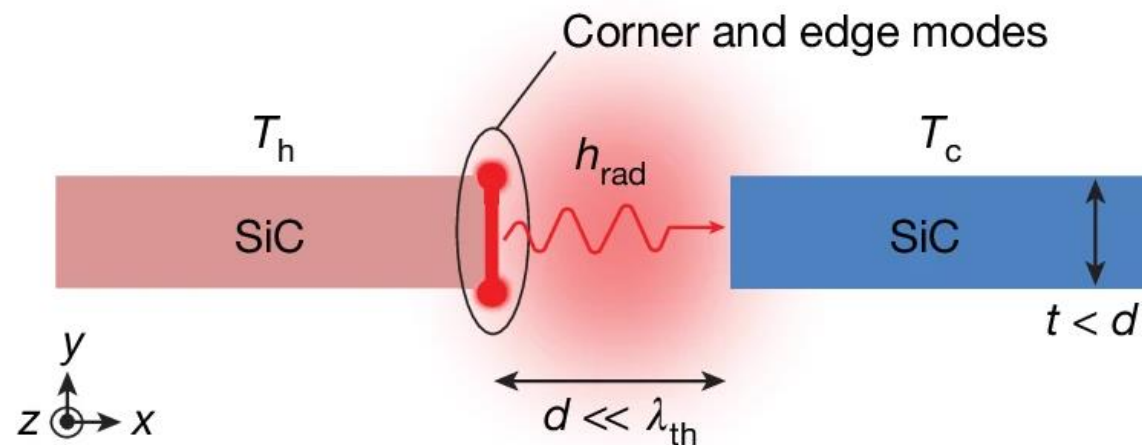


Coupled EM modes at the corners and edges of rectangular metallic membranes (non-thermal)

Berini, *Phys. Rev. B* **61**, 10494, 2000

Thermal nanophotonics in the

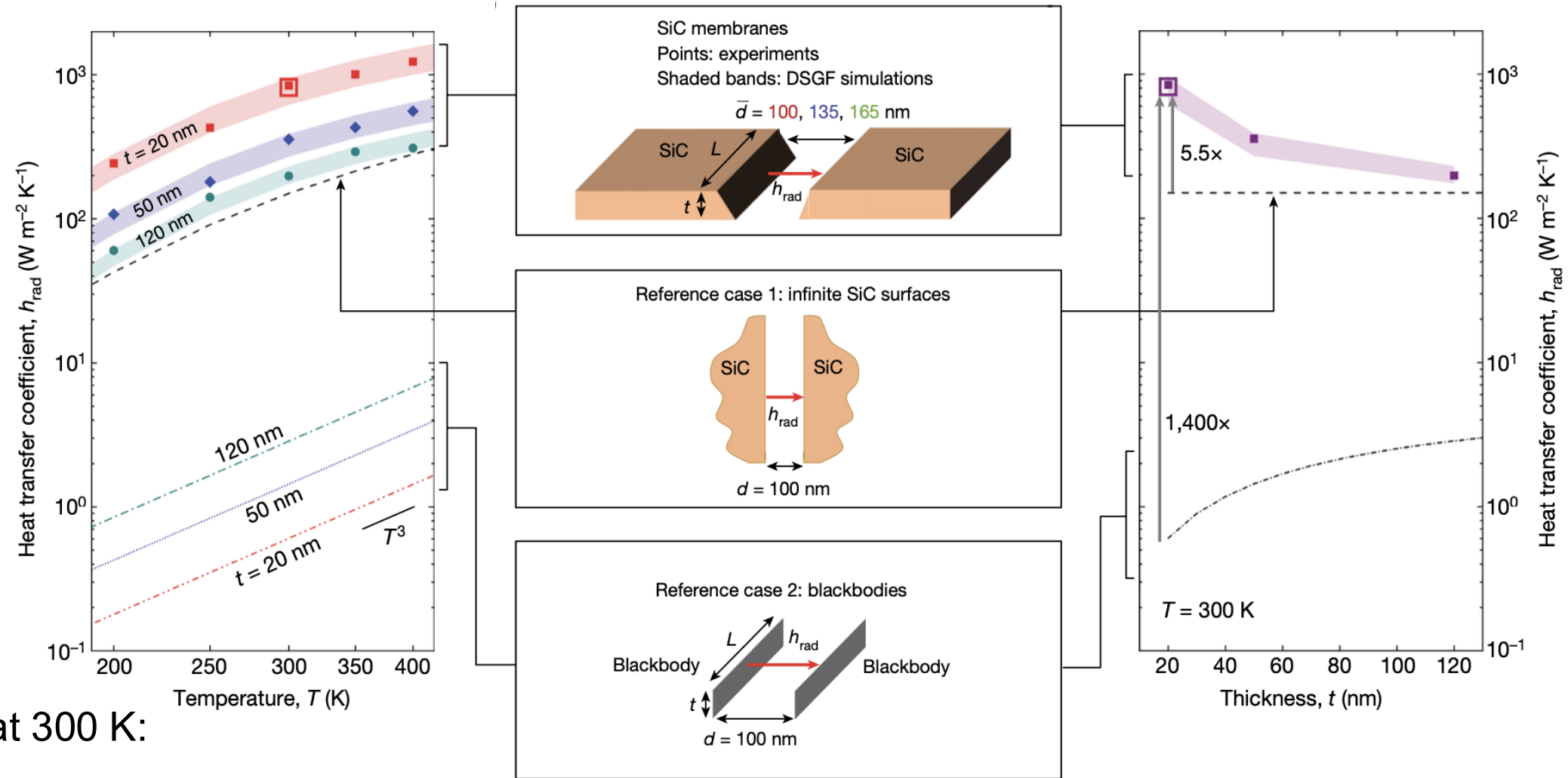
dual nanoscale regime: $t < d \ll \lambda_{\text{th}}$



Tang, Corrêa et al., *Nature* **629**, 67-73, 2024

Key finding: Near-field radiative heat transfer between SiC membranes in the dual nanoscale regime exceeds that between infinite surfaces

DSGF simulations showed good agreement against experimental results



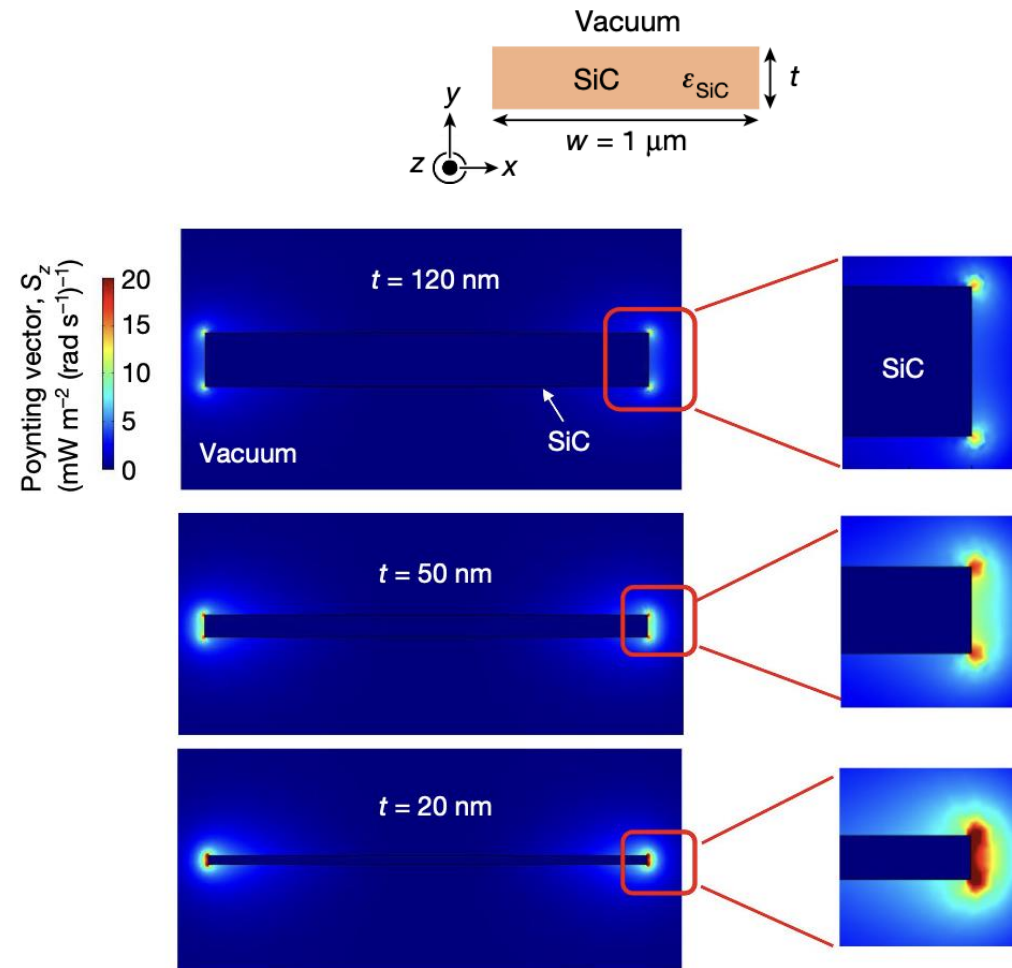
$t = 20 \text{ nm}$ at 300 K :

- $h_{\text{rad}} \sim 830 \text{ Wm}^{-2}\text{K}^{-1}$
- ~ 5.5 times larger than h_{rad} between SiC infinite surfaces
- ~ 1400 times larger than h_{rad} between blackbodies accounting for the view factor

Tang, Corrêa et al., *Nature* **629**, 67-73, 2024.

Coupling of corner and edge modes increases as t decreases

Modal analysis of a solitary SiC membrane using COMSOL Multiphysics:

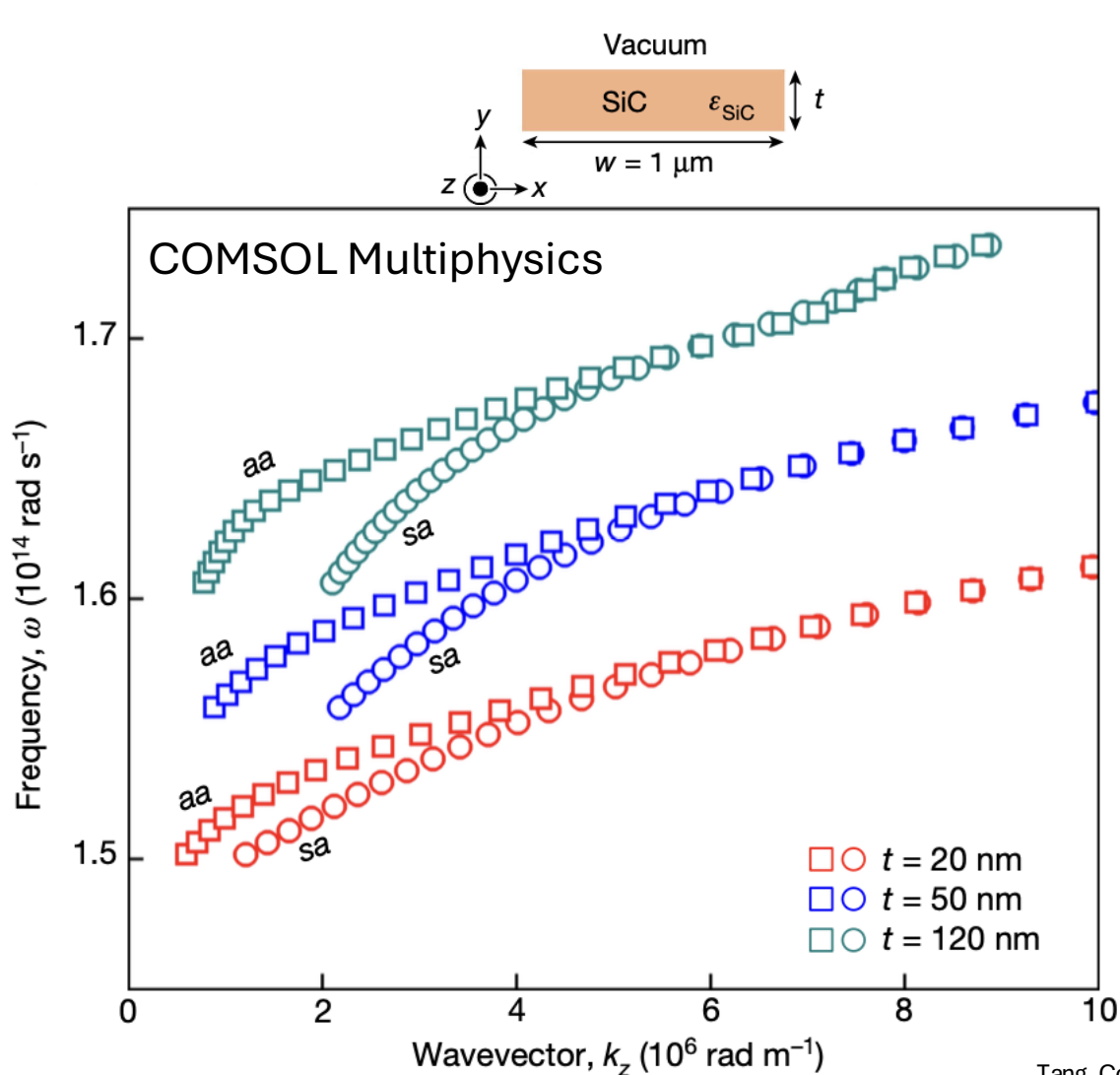


Tang, Corrêa et al., *Nature* **629**, 67-73, 2024.

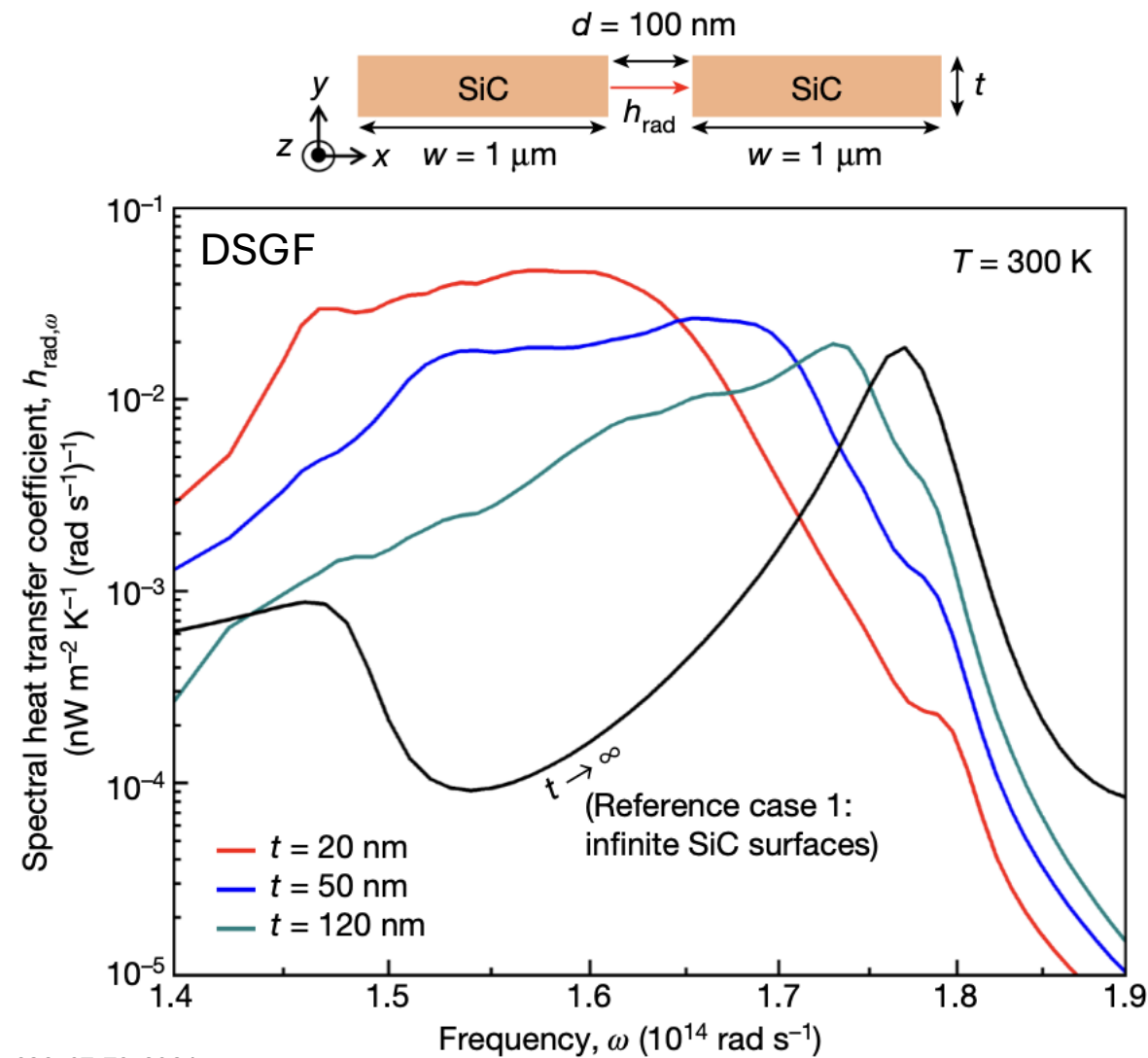
Poynting vector along z -direction showing representative corner and edge modes

The dispersion curves indicate the resonance of the heat transfer coefficient

- The maximum contributing wavevector dominating NFRHT is estimated as $\approx d^{-1} \approx 10^7 \text{ rad/m}$

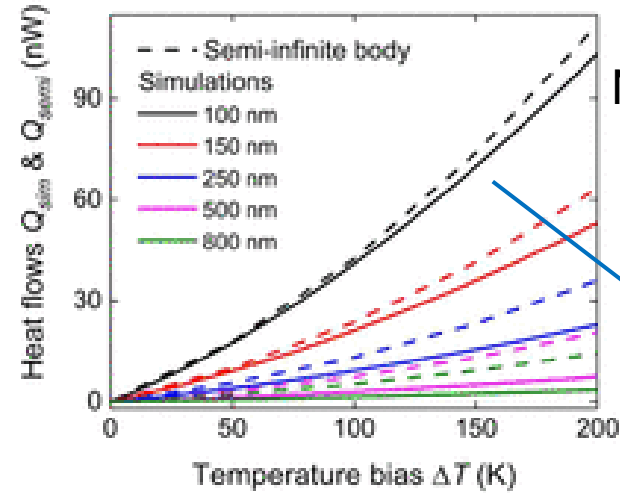


Tang, Corrêa et al., *Nature* **629**, 67-73, 2024.

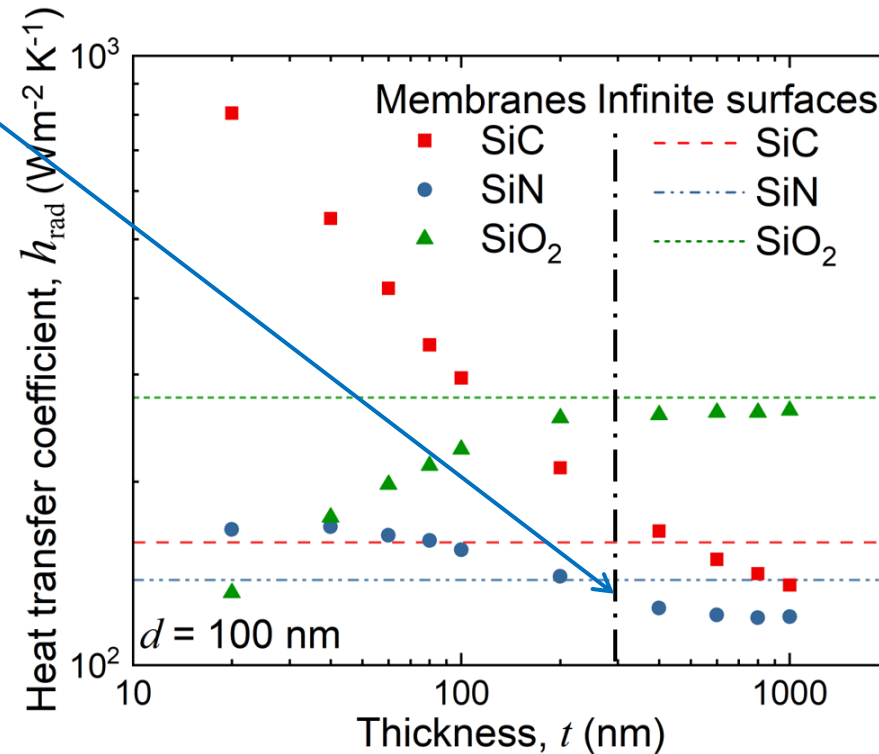


Why the heat transfer between polaritonic membranes not always surpass that of between two infinite surfaces?

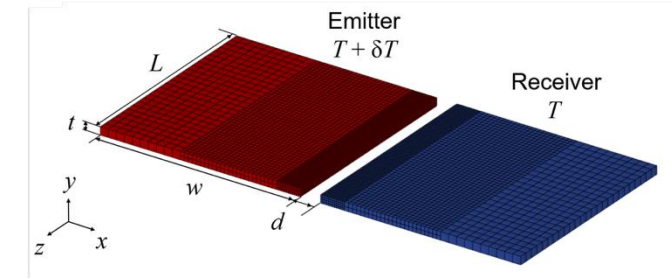
SiN with $t = 300$ nm



Numerical simulations using the DSGF solver at $T = 300$ K
for $w = 1 \mu\text{m}$, $L = 1 \mu\text{m}$, and $d = 100$ nm.

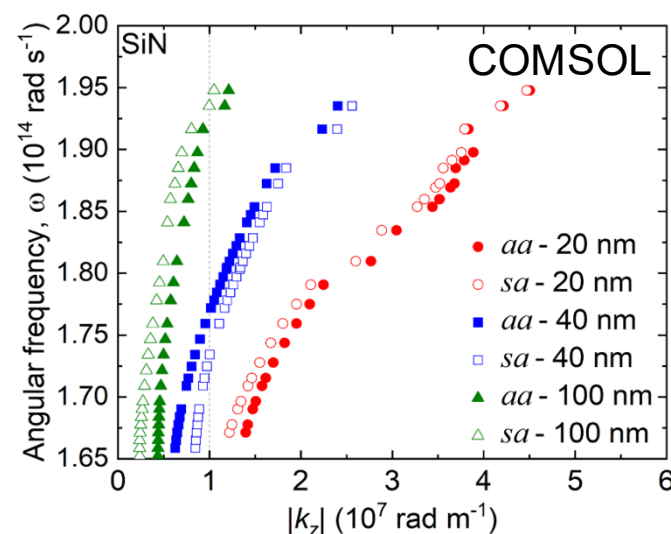
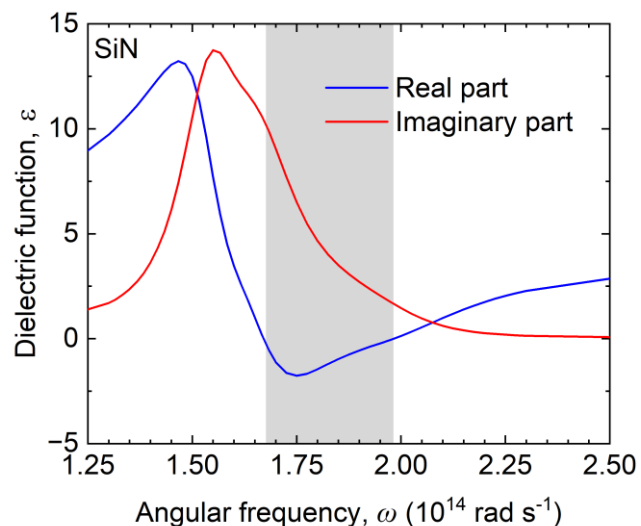
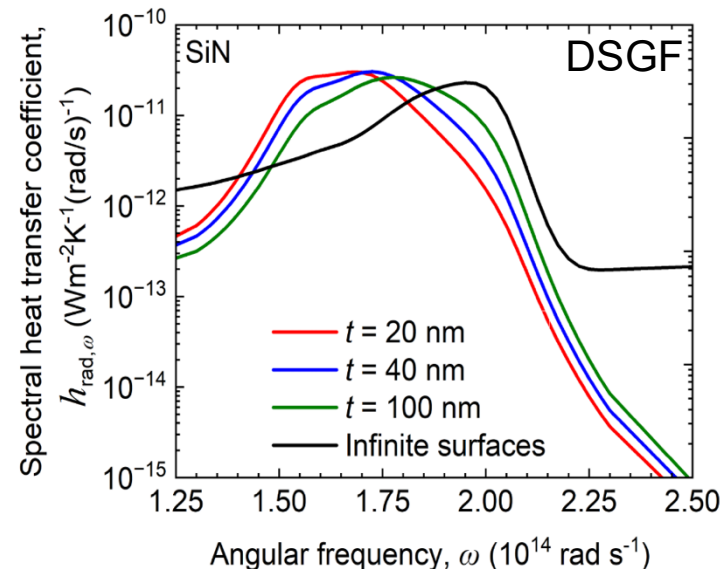
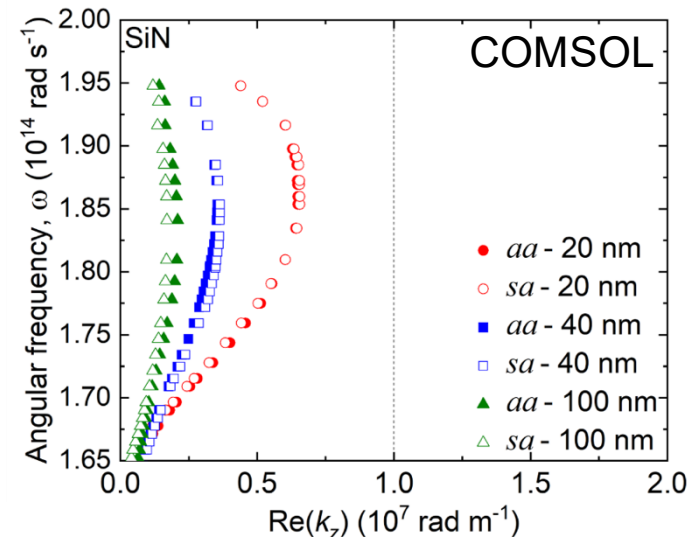


McCormack et al., *Phys. Rev. Lett.* **136**, 146303, 2026.



Key finding: Material losses play a key role enhancing or attenuating
near-field radiative heat transfer

SiN: non-negligible losses reduce the available density of states



- The maximum contributing wavevector dominating NFRHT is estimated as $\approx d^{-1} \approx 10^7$ rad/m
- **Re ($k_{z,max}$)** occurs ~at the same frequency
- Corner and edge modes induce resonance **redshift**
- SiN presents **non-negligible** material losses along the Reststrahlen band
- **$|k_z|$** should be used to indicate resonance
- For $d = 100$ nm, $|k_{z,max}| \approx 10^7$ rad/m
- For $t = 20$ nm, **Re ($k_{z,max}$) $\approx 10^6$ rad/m**
- **Re(k_z) $\ll |k_z|$**

This research resulted in two publications

Article

Corner- and edge-mode enhancement of near-field radiative heat transfer

<https://doi.org/10.1038/s41586-024-07279-2>

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Near-Field Radiative Heat Transfer in the Dual Nanoscale Regime between Polaritonic Membranes

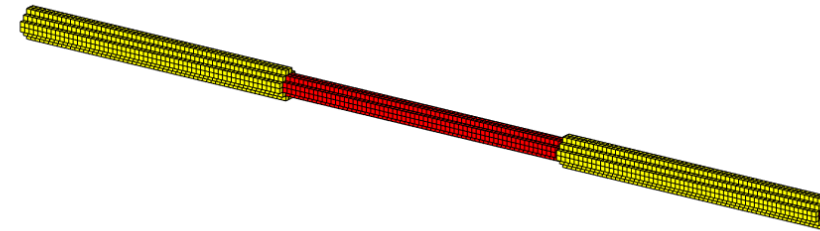
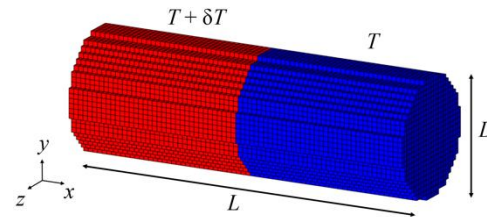
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The DSGF method enables rigorous prediction of radiation conduction in nanostructures



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Thank you! Questions?

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