Supporting Information

Design of Selective Metasurface Filter for Thermophotovoltaic Energy Conversion

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1. FDTD validation

For simulating nano-scale optical systems, the Finite-Difference Time-Domain (FDTD) approach provides a rigorous and powerful tool. The maximal problem size is limited solely by the computational power available, as FDTD solves Maxwell's equations directly without any physical approximation. The FDTD approach solves Maxwell's equations on a mesh and computes *E* and *H* at grid points spaced Δx, Δy, and Δz away in all three spatial dimensions, with E and H interlaced. Scattering, transmission, reflection, absorption, and other effects are included in FDTD. To validate the FDTD simulations in the paper, we reproduced the results of spectral emittance varying with nanowire height obtained in literature [35] as shown in Figure 28.

The following steps were followed in the Lumerical FDTD software to run the simulations:

1. The simulation region was set to the required dimensions and the injection direction was set in the positive *X* direction.
2. The *Y* and the *Z* dimensions were set to match the periodicity.
3. Next under mesh settings the mesh size (ΔX, ΔY, and ΔZ) were selected to be 5 nm.
4. To check the convergence, the mesh sizes were made finer 3 and 4nm and the results were compared.
5. It was required for the light to propagate in the *X* direction to infinity and hence a perfectly matched layer (PML) boundary was assigned.
6. Periodic boundary conditions were assigned in both *Y* and *Z* directions.
7. Plane wave light source with Bloch/ Periodic conditions was created.
8. Finally, the required geometry and the power monitors were created at required locations to get the transmittance and the reflectance of the structure.

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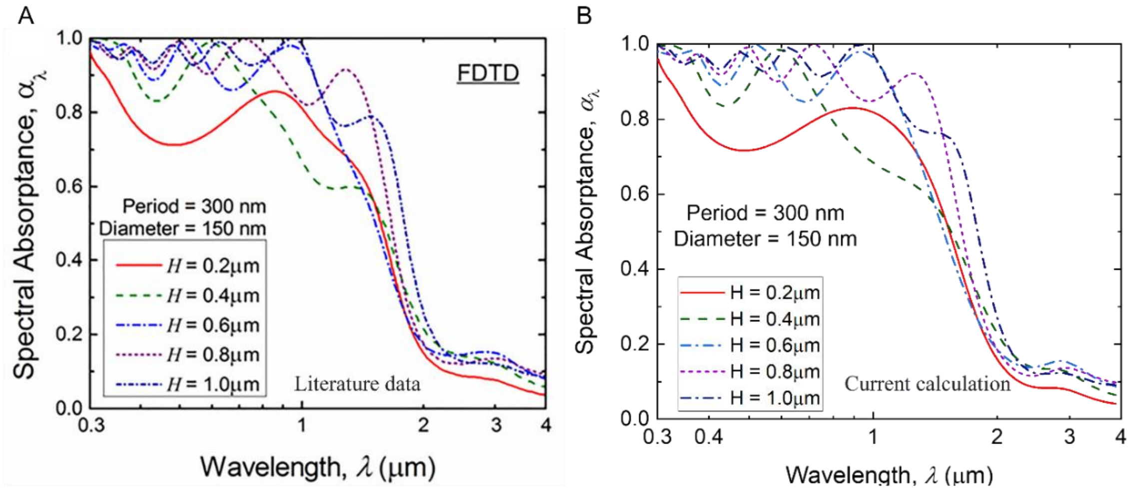

Figure S1: The spectral absorptance of the selective absorber varying with nanowire height based on FDTD simulation from (a) literature and (b) current modeling.

2. FDTD convergence check

With nonuniform meshing, a minimum mesh size of 5 nm is employed, and the numerical error is less than 1% when compared to a simulation with a minimum element size of 3 nm.

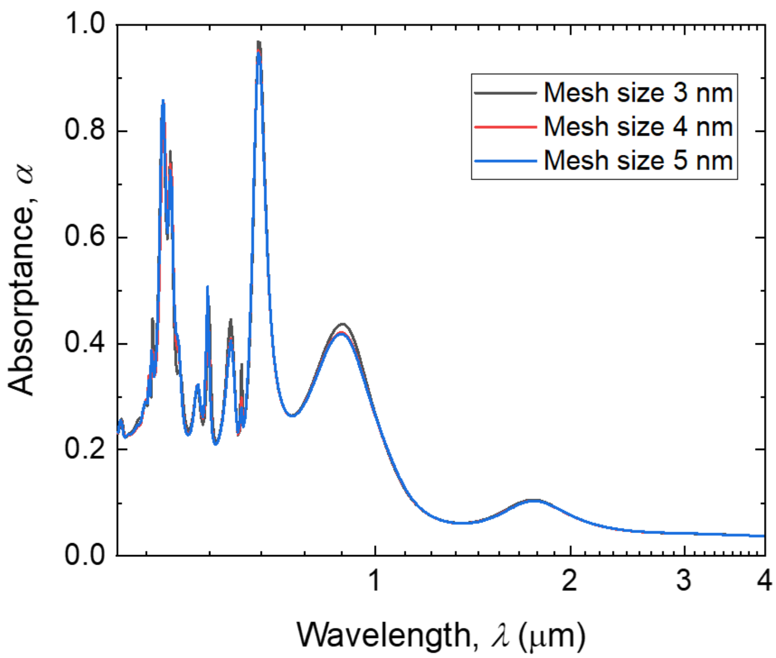

Figure S2: Convergence check for FDTD comparing the absorptance of the metasurface structure for mesh sizes of 3, 4 and 5 nm.

3. Absorption spectra of the metasurface filter with varying geometric parameters

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For reference to section 2.4 in the main text the absorption of metasurface was plotted varying with the geometrical properties of the nanopillar. The absorption plots shown in Figure S3 verify the existence of MP and the variation of MP resonance peak wavelength with geometric parameters like the diameter, heigh and the period of aluminum nanopillars on the quartz substrate.

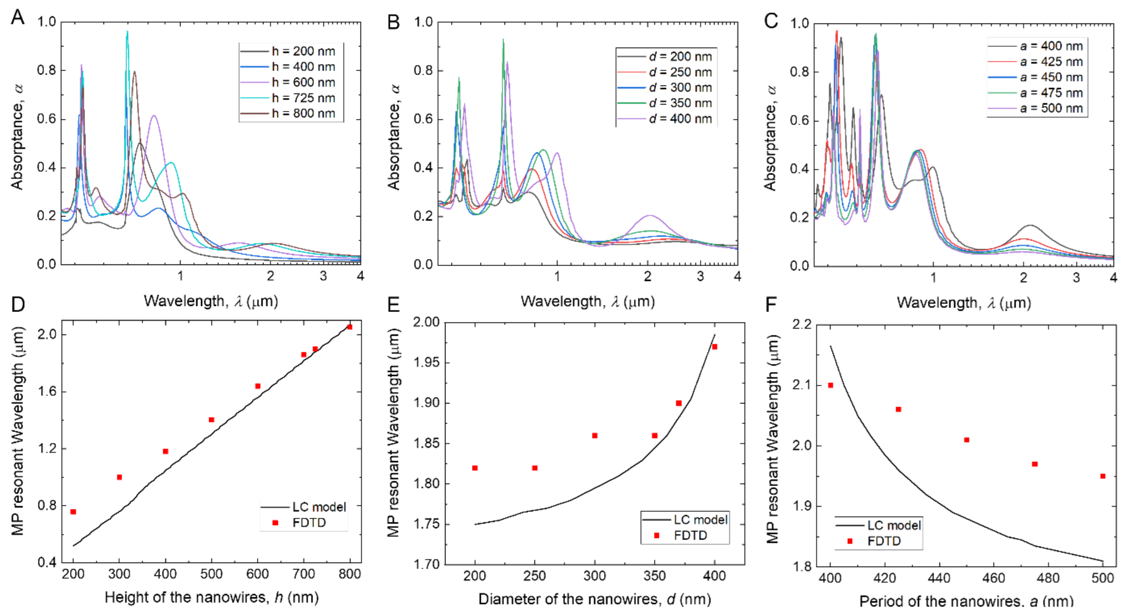

Figure S3: The spectral absorptance with respect to different nanopillars: (a) diameter, (b) height and (c) period simulated by FDTD. The MP1 wavelengths predicted by FDTD, and LC circuit model for different nanopillar parameter: (d) diameter, (e) height and (f) period.

4. Validation of TPV system efficiency calculations

The TPV system efficiency calculations were first validated by obtaining results from literature [32]. The cell IQE and absorptance obtained from Tang et al. [30] are plotted along with the refractive index (*n*) and extinction coefficient (*k*) of GaSb [45] as shown in Figure S4:

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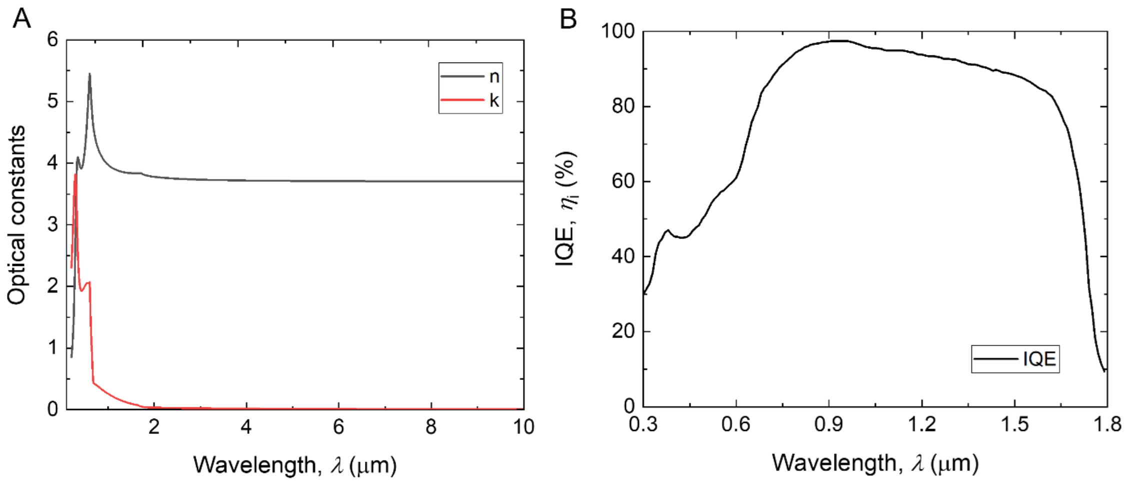

Figure S4: (a) The refractive index (*n*) and extinction coefficient (*k*) of GaSb cell obtained from Adachi. (b) The IQE of GaSb cell used in the study obtained from Tang et al.

The emitter and the cell efficiency were plotted as a function of emitter temperature for the validation using the calculation method used in this paper as shown in Figure S5.

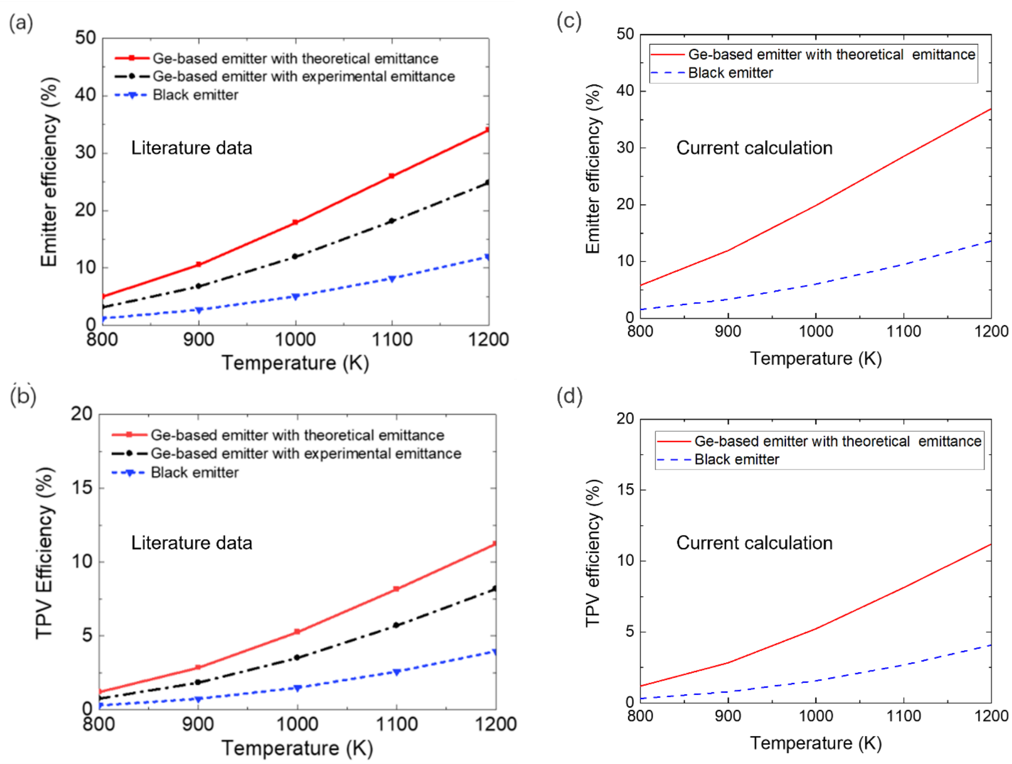

Figure S5: (a) Spectral efficiency (literature), (b) TPV efficiency (literature), (c) Spectral efficiency (current calculation) and (d) TPV efficiency (current calculation) from 800 K to 1200 K.

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5. GaSb TPV cell with different below bandgap (bbg) absorptance

The nominal value of the bbg absorptance of the cell was varied to check its effect on the cell performance parameters. Figure S6(a) & (b) show that the spectral and the overall TPV efficiency is dependent on the bbg absorptance. At low bbg absorptance, both the efficiencies improve and start decreasing with an increase in the value of absorptance below the bandgap of the GaSb cell. From Figure S6(c) we can observe that the bbg absorptance of the cell primarily affects the net radiative heat flux to the cell. Due to higher absorptance below the bandgap, the cell absorbs incoming radiation in this energy regime that does not promote the carrier generation and hence does not contribute to useful power output. Figure S6(d) shows that the power output is not varying with respect to bbg absorptance.

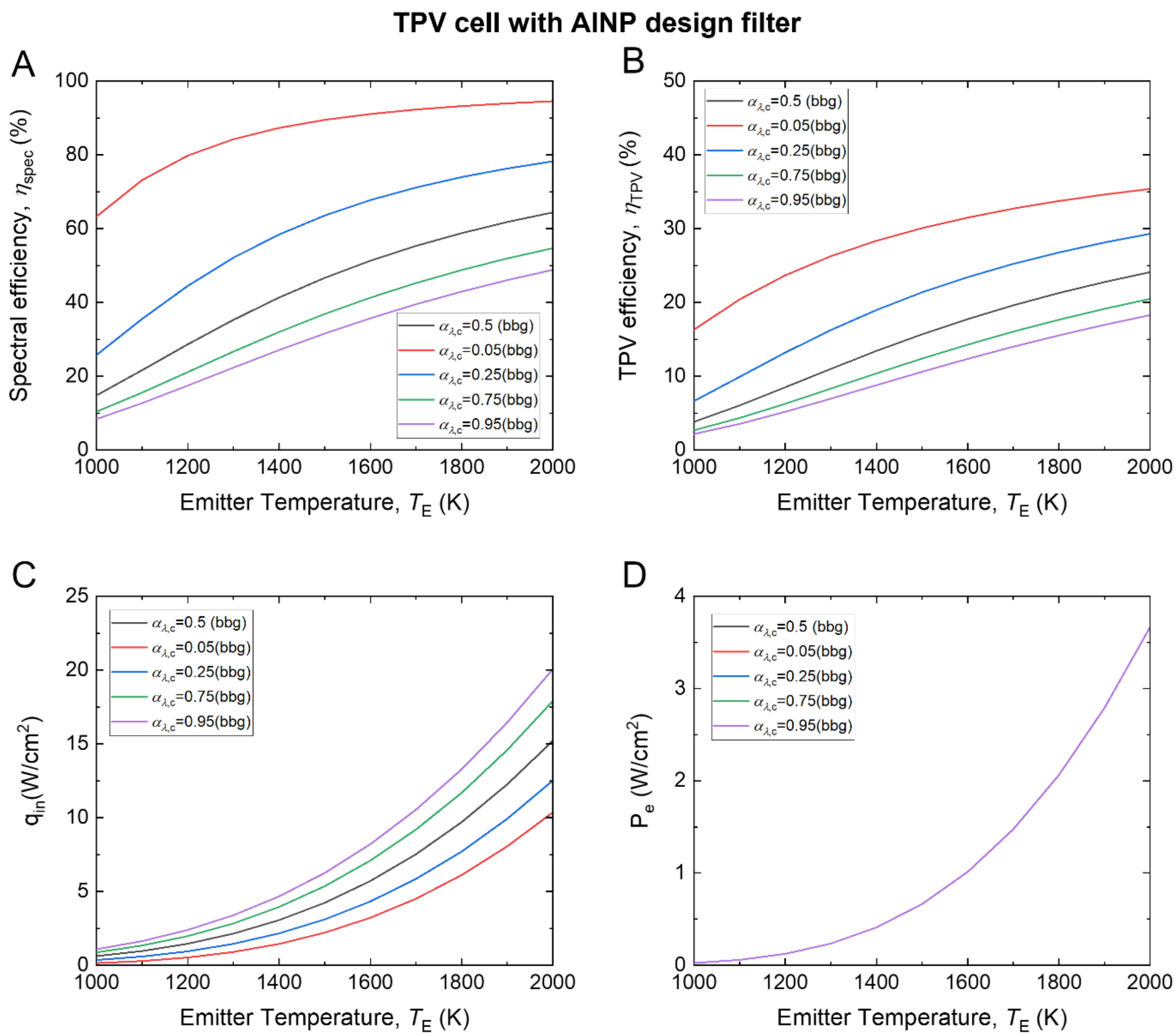

Figure S6: (a) Spectral efficiency, (b) TPV efficiency, (c) net radiative heat flux and (d) output power at different temperatures from 1000 K to 2000 K with theoretical AlNP metasurface filter, and black emitter paired with a GaSb cell for different bbg absorptance of the cell.

6. GaSb TPV cell with 100% IQE

The TPV efficiency was determined for GaSb cell with 100% IQE and compared with an actual cell. For an ideal GaSb cell with 100% IQE and the designed metasurface filter, the TPV efficiency can be further improved up to 31.1% from 24.7 % at an emitter temperature of 2000 K.

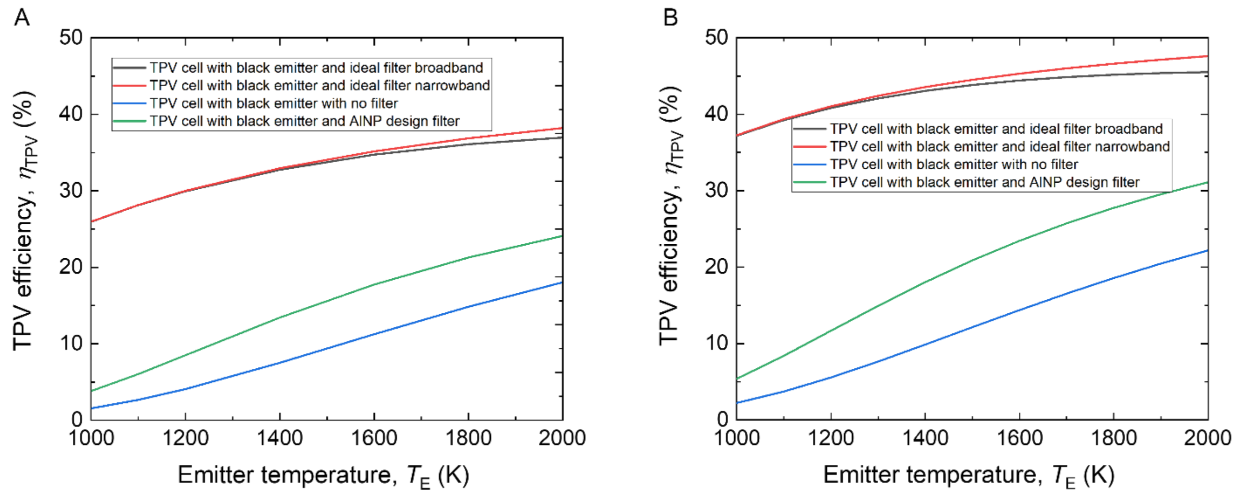

Figure S7: Calculated TPV efficiency of a GaSb cell varying with emitter temperature for an (a) actual cell and (b) ideal cell with 100% IQE.