Optimized Fabry-Pérot cavity engineered nanoscale thermoelectric generators

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Aiming to maximize the waste-heat conversion efficiency at a given output power or vice-versa, we propose a realistic design scheme of a heterostructure based superior thermoelectric generator that can give rise to an excellent trade-off between power and efficiency. On achieving the desired boxcar shaped transmission, we further explore the optimum design possibilities of Fabry-Pérot cavity structures over a central resonant tunneling diode region to maximize the area under ground state transmission. Based on our findings, we propose two new design guidelines for cavity based heat engines and demonstrate that they perform significantly better than the existing proposals in terms of boosting the output power without a cost in efficiency. It is theoretically demonstrated using the non-equilibrium Green’s function technique coupled with self-consistent charging effects that an enhancement in the output power up to 18% can be achieved at almost the same efficiency. Furthermore, an elaborate comparative study of the linear response parameters is also presented and explained in terms of the physical transport properties. This study suggests an optimal device design strategy for an improved thermoelectric generator and sets the stage for a new class of thermoelectric generators facilitated via electronic lineshape engineering.

I. INTRODUCTION

Nanostructuring of thermoelectric (TE) materials has acquired unabated precedence over their bulk counterparts [1–8] since last two decades due to their highly efficient energy harvesting capability. Over the years, research in this field was primarily focused on achieving high thermoelectric figure-of-merit by means of lineshape engineering [1–6], thermal conductivity reduction through interface engineering [9–11] and enhancement of power factor utilizing energy filtering effects [12–14]. The figure of merit concept typically assists in determining whether a material is a good thermoelectric or not. However, when actual device designs are considered, non-linear transport studies [15, 16] dealing with the trade-off between conversion efficiency and output power of the entire set up [5, 17–23] have gained precedence.

In this context, an important work by R. S. Whitney [24, 25] suggested that in a thermoelectric device set up, a boxcar type electronic transmission function of a particular bandwidth can offer optimum trade-off by maximizing the efficiency at a given power. However, practical design guidelines of such type of devices are not well addressed. Several efforts have been made after that to realize such an electronic transmission feature by proper arrangements of tunnel coupled quantum dots [15, 26].

A few recent studies utilized the miniband feature of superlattice based devices [16–18, 27] to achieve such a boxcar transmission. Further advancing on the superlattice idea, recently, thermoelectric generator (TEG) setups augmented with an electronic anti-reflection cavity (ARC) [27, 30] have been proposed using the basic thumb rule for ARC design [31]. These ideas proved to be far superior in terms of achieving excellent power-efficiency trade-off in comparison with competing device proposals [16–18, 27]. However, it should be noted that, in the presence of charging effects, the superlattice designs suffer from serious lineshape imperfections which badly affects the power and trade-off characteristics. Moreover, the large number of constituting layers in such devices poses a serious threat to the precise epitaxial growth with the existing technology. The object of this paper is to hence propose a minimal double barrier resonant tunneling (RTD) based TEG and explore its design space to provide a robust design after examining and taking into consideration all the aforementioned aspects.

Figure 1 depicts the general schematic of the cavity engineered heterostructure based thermoelectric generator setup. The central region, in general, consists of a multi period heterostructure sandwiched between two electronic cavity sections. This work considers the use of a simple double barrier resonant tunneling structure embedded by cavities of varying wall geometry to optimize the desired shape of transmission spectrum.
we have further explored the variation of the transmission probability as a function of the cavity wall geometry. It is observed that the maximum transmissivity ($TM$) which is the area under ground state transmission profile, increases along a hyperbolic path on the design plane, preserving the desired lineshape of the transmission. This result motivated us to explore various design possibilities of cavity based heat engines with even better trade-off characteristics. To investigate the thermoelectric properties, we pick two new design schemes (shown in green and red) from the design plane and it is found that the new proposals significantly enhance the power at the same efficiency and show an excellent trade-off characteristics when compared to the existing superlattice based proposals [16, 27, 30].

The rest of the paper is structured as follows. In Sec. II, the variation of the transmission function with respect to different cavity designs is thoroughly examined and based on the results two new practical design schemes are proposed. The band schematics of all the devices are depicted in Sec. III with a clear description of the physical properties. Section IV briefly discusses the simulation setup and illustrates the formalism used. In Sec. V, the results are thoroughly discussed in terms of all the performance parameters and a detailed comparative study is presented in order to highlight the improvements achieved through our new proposals. We conclude the paper in Sec. VI.

II. TRANSMISSION FUNCTION

In this section, we closely inspect the variation of the transmission function, $T(E)$, with respect to the stoichiometric and geometric changes of the cavity wall. The thumb rule of designing ARC says that the wall width ($b_{FP}$) and height ($h_{FP}$) of the cavity region should exactly be half and equal, respectively, to that of the central barrier region [31]. Although, one should always ponder that the combined effect of $b_{FP}$ and $h_{FP}$, plays a crucial role on tailoring the lineshape of the transmission. We note that the amount of aberration from the band-pass nature caused by a tiny reduction in $b_{FP}$, can be overly compensated by a proportional increment in $h_{FP}$. This finding calls for a further investigation on the possible betterment of the boxcar nature of the transmission by means of optimal cavity engineering. A quantitative measure in this regard is the transmissivity ($TM$) which is the area under the transmission function corresponding to the lowest energy state, given by

$$TM = \int_0^{E_1} |T(E)| \, dE,$$

where the energy $E_1$ is chosen in such a way that it falls almost in between ground and first excited state with a zero transmission probability. Figure 2(a) displays the variation of $TM$ as a function of $b_{FP}$ and $h_{FP}$ in a gray scale color plot. We observe that $TM$ exhibits a nearly hyperbolic trend around its maxima which monotonically increases (along the direction of the black dotted arrow) with decreasing $b_{FP}$ and increasing $h_{FP}$. This result, although indicates an improvement in the area under transmission, but never delineates its actual shape. We, therefore, pick two new design schemes of the FP cavity namely, FP-II (green diamond) and FP-III (red star) as indicated in Fig. 2(a) alongside the ARC (FP-I) based proposal (blue circle) [30, 32] for further investigation. The equilibrium transmission function of all the cavity based devices are shown as a function of energy. The peaked transmission of the central RTD region (without the ARC) is also shown here to emphasize the role of cavity engineering on transmission.

FIG. 2. Transmission function: (a) Ground state transmissivity is shown in a gray scale color plot as a function of the cavity wall width and height. The locus of its maxima follows a hyperbolic trend which increases along the direction of the black dotted arrow. Two new design schemes are picked (green and red) for further investigation and comparison with the ARC based proposal (blue). (b) Equilibrium transmission function of all the cavity based devices are shown as a function of energy. The peaked transmission of the central RTD region (without the ARC) is also shown here to emphasize the role of cavity engineering on transmission.
ARC based design which might cost the efficiency a bit at the lower values of contact Fermi level. It is also important to note that the cavity region is designed in such a way that it pulls the transmission minima to unity at a particular design energy, which might not be the mid-band energy always. In this case, the band spectra suggest that the design energies corresponding to the new proposals move above the central peak unlike a typical ARC based structure [30].

III. DEVICE SCHEMATIC AND DESCRIPTION

The physics of ARC is now well established and explained elaborately in terms of the electronic Bloch states in the neighborhood of the peak transmission energy [30, 31, 33, 34]. In this work, in a more generic way, we use the term Fabry-Pérot cavity as there is no fixed design rule of the cavity to utilize the anti-reflective feature. The interplay between the width and height of the cavity wall has a major role to play here on preserving the band-pass nature of the transmission. It is intuitively understood that the undesired effect of lineshape sharpening caused due to lowering of the wall width can be largely restored to its original band-pass form by a proportional increment of the wall height. One thus always has the freedom to engineer the cavity region within the fabrication capabilities.

Based on the design rules discussed in the last section, we depict the conduction band schematics of all the three cavity engineered devices (FP-I, FP-II and FP-III) along with the standard RTD device. These devices are having an ideal infinite extent in the transverse direction with a finite length along their transport direction (here, z-direction). The central RTD structure, as shown in Fig. 3(b), is modeled with a GaAs well of width \( w = 4.2\text{nm} \) in between two \( Al_xGa_{1-x}As \) barrier of width \( b = 2.4\text{nm} \), where \( x \) is aluminum mole-fraction. Barrier height is kept fixed at \( 0.3eV \) with respect to the well by precisely tuning the mole-fraction parameter. These design parameters are chosen in accordance with a realistic ground state transmission FWHM of \( k_BT/2 \), where \( k_B \) is the Boltzmann’s constant and \( T \) denotes the temperature. For the cavity based devices, the same RTD structure is symmetrically placed within the cavity regions such that the width of the well region between any two successive barriers remains the same at \( w \). However, the varying design of cavity wall gives rise to different structures as listed below:

- In Fig. 3(c), FP-I: \( h_{FP} = h \) and \( b_{FP} = b/2 \),
- In Fig. 3(d), FP-II: \( h_{FP} = 3h/2 \) and \( b_{FP} = 3b/8 \),
- In Fig. 3(e), FP-III: \( h_{FP} = 2h \) and \( b_{FP} = b/4 \).

The devices described above can be fairly accurately modeled using a nearest neighbor tight-binding Hamiltonian of a linear atomic chain within the single-band effective mass approximation [39]. The GaAs/AlGaAs material system is chosen here due to its less variability of effective mass over a wide range of composition and excellent lattice matching capability. Using the non-equilibrium Green’s function (NEGF) technique coupled with the charging effect, we present a comparative study of the devices discussed above in terms of the linear and non-linear thermoelectric performance parameters. The device dimensions used here are in the order of the relaxation length scales which eliminates the possibility of scattering to ensure a coherent transport of carriers.
within the ballistic limit [17]. On the other hand, the presence of nano-structured interfaces strongly restricts the flow of phonons in the device. This implies that the heat current flowing through the device is mainly due to electrons. Therefore, the lattice contribution to the thermal conductivity is ignored here.

The cavity-based devices manifest high immunity to the non-equilibrium changes in transmission function due to the charging effect. This results in an improved trade-off characteristics for a wide range of contact Fermi level. Furthermore, the widening of the transmission window allows a large number of additional transverse modes to conduct and contribute to the net charge current which in turn boosts the power. Based on the results, we can definitely assert that the width of the transmission function obtained here is still below the ideal theoretical limit predicted by Whitney [24] which makes a room for further research.

IV. SIMULATION METHODOLOGY AND SETUP

Figure 3(a) shows a typical voltage-controlled thermoelectric heat engine setup [36] which will be used throughout for the purpose of simulation. The flow of electrons due to the thermal driving force from the hot to cold contact is opposed by the voltage drop across the load resistance connecting them. The polarity of this drop is such that it lowers the quasi Fermi level of the hot contact with respect to the cold contact which, as a result, causes an opposite flow of electrons. In the simulation framework, the variation of the load resistance is incorporated through the application of a positive voltage at the hot contact end.

The simulation methodology is mainly divided into two important parts, namely, (i) self-consistent estimation of the electronic transmission spectrum of the test device and (ii) the calculation of charge and heat currents from the knowledge of the obtained transmission function. For the former part, we utilize the standard atomistic NEGF formalism self-consistently coupled with the Poisson equation. In order to analyze the device behavior under different operating conditions, we vary the equilibrium quasi Fermi levels \( E_f \) of the hot \((\mu_H)\) and cold \((\mu_C)\) contacts. For a given applied bias of \( V_{app} \), the Fermi level of the hot (cold) contact is shifted downward (upward) from its equilibrium value by an amount of \( qV_{app}/2 \) due to symmetric electrostatic coupling, where \( q \) is the unit electronic charge. The simulation begins with a linear potential profile as an initial guess to calculate the longitudinal energy \( E \) resolved retarded Green’s function \( G(E) \), given by

\[
G(E) = [(E+i0^+)] - H - U(z) - \Sigma_H(E) - \Sigma_C(E)]^{-1}, \tag{2}
\]

where \( U(z) \) is the potential profile along the transport direction, \( \Sigma_H(C) \) is the self-energy matrix of the hot (cold) contact and \( \mathbb{1} \) is the identity matrix. Having obtained \( G(E) \), the carrier concentration \( n \) can be easily calculated from the electron correlation function, \( G^n(E) \), which is then fed into the Poisson’s equation to calculate the updated potential profile. The set of equations governing the above-mentioned routine are given by

\[
G^n(E) = G[\Gamma_H f_{2D}(\mu_H) + \Gamma_C f_{2D}(\mu_C)]G^\dagger, \tag{3}
\]

\[
n = \frac{1}{\Delta z} \int \frac{G^n(E)}{2\pi} dE, \tag{4}
\]

\[
d^2\mu(E(z)) = -\frac{q^2}{\epsilon_0\epsilon_r} n \tag{5}
\]

where \( \Delta z \) is the discrete lattice spacing parameter, \( \epsilon_0 \) is the free space permittivity, \( \epsilon_r \) is the relative permittivity of GaAs which is assumed to be uniform throughout the lattice and \( \Gamma_{H(C)} \) represents the broadening function of hot (cold) contact. The contribution from all the transverse modes are encapsulated in the \( f_{2D} \) function which is defined as [35]

\[
f_{2D}(E - \mu) = \frac{m^* k_B T}{2\pi\hbar^2} \log[1 + \exp\left(\frac{\mu - E}{k_B T}\right)], \tag{6}
\]

where \( h \) is the reduced Planck’s constant and \( m^* \) is the electron effective mass which is also considered to be uniform throughout the lattice. For our simulations, we take a constant effective mass of 0.07\( m_0 \) across structures, where \( m_0 \) is the free electron mass. Above procedure is performed self-consistently until the convergence is achieved and the non-equilibrium transmission function, \( T(E) \), can thereby calculated as

\[
T(E) = Tr[\Gamma_H \Gamma_C G G^\dagger]. \tag{7}
\]

The resultant transmission function is then fed into the NEGF current formula to calculate the charge \( J \) and heat current \( (J^Q) \) densities [35]. Summing over all the current carrying transverse modes and absorbing that in the \( f_{2D} \) function, total charge current flowing through the device is given by

\[
J = \frac{q}{\pi\hbar} \int dE T(E) [f_{2D}(E - \mu_H) - f_{2D}(E - \mu_C)]. \tag{8}
\]

It is important to note that the total heat current which is the energy weighted charge current, is resolved into two components namely, \( J_H^Q \) and \( J_H^Q \) based on the contributions from longitudinal and transverse energy degrees of freedom, respectively. Therefore, the total heat current flowing through the hot contact \( (J^Q_H) \) is expressed as \( J_H^Q = J_H^{Q1} + J_H^{Q2} \), where \( J_H^{Q1} \) and \( J_H^{Q2} \) are given by

\[
J_H^{Q1} = \frac{1}{\pi\hbar} \int dE T(E)(E - \mu_H)
\times [f_{2D}(E - \mu_H) - f_{2D}(E - \mu_C)], \tag{9}
\]
where \( g_{2D} \) function is defined as [17, 30]

\[
g_{2D}(E - \mu) = \frac{m^*k_B T}{2\pi\hbar^2} \int_0^\infty \frac{d\epsilon_{\perp}}{1 + \exp\left(\frac{E + \epsilon_{\perp} - \mu}{k_B T}\right)}. \tag{11}
\]

The integration in Eq. (11) is performed numerically where the upper limit of energy is chosen high enough to include all the significant transverse modes. We assume a parabolic dispersion relation \((\epsilon_{\perp})\) in the transverse direction and the integration over all the momentum \((\vec{k}_{\perp})\) eigenstates is carried out with a periodic boundary condition.

Once the charge \((J)\) and heat current \((J_H^Q)\) densities are calculated, the output power density \((P)\) and conversion efficiency \((\eta)\) can be obtained using the standard thermoelectric setup [39] by the following relations

\[
P = JV_{\text{app}}, \tag{12}
\]

\[
\eta = P/J_H^Q. \tag{13}
\]

The efficiency is usually measured as a ratio to that of the Carnot’s limit \((\eta_C)\), defined as \(\eta_C = 1 - T_C/T_H\)

The allowed range of power restricts the device operation between short circuit \((V_{\text{app}} = 0)\) to open circuit \((V_{\text{app}} = V_{\text{OC}})\) condition, where \(V_{\text{OC}}\) is the open circuit voltage.

V. RESULTS AND DISCUSSION

In this section, a comparative study of the results are discussed in terms of the non-linear and linear response parameters.

A. Non-linear Response Analysis

Power and Efficiency: In Fig. 4(a) output power density (power per unit area) of all the configurations are displayed as a function of \(V_{\text{app}}\) and contact \(E_f\) in a gray scale color plot. It can be seen that the power starts to increase from the short circuit condition with increasing \(V_{\text{app}}\) and reaches a local maxima before falling to zero at the onset of the open circuit condition. Strictly speaking, net current actually reverses its direction at \(V_{\text{OC}}\) and therefore the setup can’t be used as a generator beyond this point. Usable power in the region beyond \(V_{\text{OC}}\) is thus treated as zero. This trend is almost similar irrespective of the design scheme, but, what is important to note here is the variation of power with \(E_f\). When \(E_f\) moves in the vicinity of the higher excited states. But, we restrict our study only within the contribution of the ground state as the excited states hardly contribute to the conduction due to their less occupancy and is thus kept out of consideration. We, therefore, set the range of \(E_f\) between 0 – 10\(k_B T\) in our simulation.

Figure 4(a) displays the power density profile of the RTD-TE device which reveals that the maximum power of 0.49\(MW/m^2\) can be delivered at \(E_f = 4.5k_BT\). It is also important to observe that with increasing \(E_f\), \(V_{\text{OC}}\) sharply falls due to the sharp nature of the transmission and therefore the power remains non-zero only for a narrow region of operation. On the other hand, the cavity based devices due to their band-pass nature of transmission, manifest a huge improvement in the power along with a broad spectrum as depicted in Fig. 4(b), (c), (d) for the configurations FP-I, FP-II and FP-III, respectively. Obtained results show that FP-II and FP-III designs can generate maximum power \((P_{\text{max}})\) up to 1.03\(MW/m^2\) and 1.06\(MW/m^2\), respectively, as compared to 0.9\(MW/m^2\) of the ARC based proposal (FP-I). The position of \(P_{\text{max}}\) of the new proposals is at \(E_f = 5.5k_BT\) which is slightly higher than that of
FIG. 5. Comparative study of efficiency: Conversion efficiency normalized to Carnot’s efficiency of (a) RTD, (b) FP-I, (c) FP-II, and (d) FP-III devices are shown as a function of applied bias and contact $E_f$. The efficiency in general becomes maximum in the close proximity of $V_{OC}$ at $E_f = 0$. The cavity based new proposals show almost similar range of efficiency with a hint of improvement in the maximum value as compared to the ARC based device.

the RTD-ARC device (FP-I) whose $P_{max}$ occurs at $E_f = 5k_BT$. This result is in good agreement with the nature of the obtained transmission functions of the new designs as they are marginally shifted upward in energy when compared to that of FP-I. One must note that deploying the new design schemes, $P_{max}$ can be boosted up to 18% over the ARC based proposal.

A device can only be qualified as a good heat engine if it can deliver considerable amount of power at a high conversion efficiency. Therefore, an important parameter to judge here is the conversion efficiency which dictates the ability of a generator to convert heat into electricity. Normalized conversion efficiency of all the devices are shown in Fig. 5 as a function of $V_{app}$ and contact $E_f$. It is seen that the efficiency becomes maximum in the close vicinity of $V_{OC}$ at $E_f = 0$ irrespective of the design scheme and decreases monotonically afterwards with increasing $E_f$. However, theoretically the efficiency can be further improved towards the ideal Carnot’s limit at the cost of generated power by pushing $E_f$ way down the conduction band edge. But those devices would hardly be of any practical use due to their poor load driving capability. Ideally, the heat current increases when the conduction takes place at higher energies. Therefore, the efficiency attains its maximum value when $E_f$ is minimum. The highest efficiency that can be achieved in the RTD-TE device is 61.5% at $E_f = 0k_BT$ as shown in Fig. 5(a). On the other hand, the cavity based devices although possessing wide transmission spectra, can offer even better efficiency due to their nearly perfect boxcar nature of transmission as evident from Fig. 5(b), (c), (d) for FP-I, FP-II and FP-III, respectively. The maximum attainable limit of efficiency that can be achieved through optimal cavity engineering is 64.4% for the aforementioned range of power. Obtained results clearly point towards an improved power-efficiency trade-off characteristics which will be discussed below.

Power-efficiency-product and Trade-off: So far, we have quantitatively discussed about the maximum achievable limit of the power and efficiency and their

FIG. 6. Comparative analysis: (a) $PEP_{max}$ and (b) $P_{max}$ are plotted with respect to different $E_f$ for all the cavity engineered devices. The difference in the range of $E_f$ pertaining to the maximum values of $PEP_{max}$ and $P_{max}$ directly point towards the trade-off between power and efficiency. It is also worth mentioning that as we move forward in the design order as in Fig. 2(a), we achieve even more improved power and $PEP$.

FIG. 7. Comparative analysis of power-efficiency trade-off along the locus of (a) $P_{max}$ and (b) $PEP_{max}$ for all the cavity engineered devices. It is noted that in both the cases the new design schemes enclose a larger area on the power-efficiency plane which allows them to operate over a long range of contact $E_f$. 
region of occurrence. We note that the variational trends followed by them are completely different in nature. But to design an efficient heat engine, one must be extremely careful in choosing the regime of operation such that the device can deliver significant amount of power at a high efficiency. In this context, instead of looking into the power and efficiency separately, their product \( \text{(PEP)} \) becomes more meaningful to inspect. For each value of \( E_f \), the maximum of \( \text{PEP} \) with respect to the applied voltage is shown as a function of varying \( E_f \) in Fig. 6(a). Besides, we also plot \( P_{\text{max}} \) with respect to \( E_f \) in Fig. 6(b) in order to compare with \( \text{PEP}_{\text{max}} \). We notice that the maximum of \( \text{PEP}_{\text{max}} \) occurs around \( E_f = 4k_B T \) which is well ahead to that of \( P_{\text{max}} \) which becomes maximum around \( E_f = 5.5k_B T \). This clearly signifies that the efficiency falls rapidly with increasing \( E_f \) which is also evident from the sharp fall of \( \text{PEP}_{\text{max}} \) beyond its maxima in contrast to \( P_{\text{max}} \). It is also worth mentioning that the margin of improvement in both the parameters becomes maximum around their respective maxima which further improves the trade-off.

We now shift our attention to the best operating regimes of these devices based on the design goals. Adhering to the commercial design standards, we thoroughly examine the power efficiency trade-off at the maximum values of power and \( \text{PEP} \) for the entire range of operation. For every value of \( E_f \), power versus efficiency is plotted along the locus of \( P_{\text{max}} \) and \( \text{PEP}_{\text{max}} \) on the power-efficiency loops as shown in Fig. 7(a) and (b), respectively. It is seen that the trade-off curves of FP-II and FP-III are almost similar in nature and enclose a large area as compared to FP-I which indicates their wide range of operation. Results signify that the best operating regime should lie in the range of \( E_f \) between 4 - 6\( k_B T \) based on the specific design requirements.

### B. Linear Response Analysis

Using the same simulation framework, the linear response parameters can be extracted from the coupled charge and heat current equations, given by

\[
I = G \Delta V + G_S \Delta T, \quad I_Q = G_P \Delta V + G_Q \Delta T,
\]

where, \( G, G_S, G_P, G_Q \) are related to the corresponding Onsager coefficients \([36]\). \( \Delta V \) and \( \Delta T \) are the applied electrical and thermal bias, respectively, which are kept small enough to ensure linear operation.

**Power Factor and Seebeck Coefficient:** Power factor \((PF)\) is defined as \(PF = S^2 G\), where \( G \) is the electrical conductivity and \( S \) is the Seebeck coefficient which is given by, \( S = -G_S/G \). In Fig. 7(a), one can easily notice the sharp and steady rise of \( PF \) beyond \( E_f = 2k_B T \) as we move higher in the design order and the maximum improvement in \( PF \) that can be achieved through optimal cavity engineering over that of the ARC based design is nearly 20% in the range of \( E_f \) between 5 - 6\( k_B T \). This result actually points towards a monotonic improvement of \( G \) as the Seebeck coefficients of the cavity based devices remain almost same for the entire range of \( E_f \) as depicted in Fig. 8(b). We understand that the marginal improvement in the transmission function although does not affect the \( \text{VOC} \) much, but accounts for considerable gain in the \( PF \) due to the additional large number of transverse current carrying modes participate in conduction.

**Figure-of-Merit:** Although the main goal of this work is to improve the non-linear performance, however, it is customary to discuss the dimensionless Figure-of-
TABLE I. Comparative study of key performance parameters.

| Device Configuration | RTD   | FP-I  | FP-II | FP-III |
|----------------------|-------|-------|-------|--------|
| $P_{\text{max}}$ (MW/m$^2$) | 0.49  | 0.90  | 1.03  | 1.06   |
| $\eta_{\text{P}_{\text{max}}}$ (%) | 44.66 | 46.34 | 46.42 | 46.32  |
| $\eta_{\text{max}}$ (%) | 61.5  | 64.1  | 64.4  | 64.4   |
| $PEP_{\text{max}}$ (MW/m$^2$) | 0.18  | 0.37  | 0.41  | 0.42   |
| $PF_{\text{max}}$ | 2.20  | 4.03  | 4.62  | 4.82   |
| $zT_{\text{max}}$ | 13.37 | 14.98 | 15.57 | 15.09  |
| $zT_{4-6k_B T}$ (mV/K) | 1.54-3.08 | 2.99-4.49 | 2.92-4.51 | 2.93-4.51 |
| $S_{4-6k_B T}$ (mV/K) | 0.15-0.21 | 0.2-0.25 | 0.2-0.25 | 0.2-0.26 |

Merit ($zT$) in order to judge the device ability as an efficient heat engine. In our study, we restrict ourselves to the electronic part of heat conduction neglecting the phonon contribution. The presence of nano-structured interfaces strongly hinders the phonon transport through the lattice which in turn results in a negligible thermal conductivity in contrast to its electronic counterpart. With these assumptions, $zT$ can be expressed as

$$zT = \frac{PF}{G_{K,el} T},$$

where $G_{K,el}$ is the open circuit electronic thermal conductivity, given by $G_{K,el} = G_Q - G_p G_S/G$. Figure 9(a) plots the $zT$ of all the devices as a function of $E_f$ which clearly reveals that the boxcar feature of the transmission significantly enhances the $zT$ throughout when compared to its peaked nature. This result is also in line with the variation of efficiency at maximum power ($\eta_{P_{\text{max}}}$) as depicted in Fig. 9(b). It is observed that in the cavity based devices, the achievable limit of $\eta_{P_{\text{max}}}$ varies in between $35-45\%$ within the allowed range of $E_f$ which is pretty high in comparison to a RTD or quantum dot based device [17]. One must also note that the range of $zT$ is almost similar in all the cavity based devices which dictates that the heat conversion ability does not degrade with an associated rise in output power. A close look on the obtained result reveals that the steady improvement of $PF$ from FP-I to FP-III is mostly suppressed by an equal rate of increase in the thermal conductivity, thereby maintaining a uniform $zT$.

The results discussed in the above sections are quantitatively summarized in Table I for a detailed comparative study of all the devices. This study would also help in designing suitable TE heat engines according to the specific output goals.

VI. CONCLUSION

In conclusion, we have vastly explored the different design features of the Fabry-Pérot cavity over the RTD structure on achieving a nearly perfect bandpass electronic transmission. We observe that the boxcar feature improves along a hyperbolic path on the cavity design plane which led us to pick two new proposals with a foresight to enhance the thermoelectric power further without compromising with the efficiency. Using the NEGF-Poisson formalism, we have presented a detailed comparative study of the linear and non-linear performance parameters in order to justify the superiority of the new proposals. Obtained results reveal that employing the new design schemes, net deliverable power can be improved up to 18% from the previous ARC based proposal at the same efficiency leading to an excellent trade-off between them. It is also noted that in the linear response regime, the steady improvement of power factor does not lead to a consequent degradation in the Figure-of-merit and the Seebeck coefficient. Furthermore, we have also discussed the operational regimes of these devices based on the margin of improvement and specific design criteria. We believe that our study opens up a new avenue on designing lineshape engineered solid state devices for various applications with the simplest of structures that can be fabricated within the existing technological framework.

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[1] L. D. Hicks and M. S. Dresselhaus, Physical Review B 47, 727 (1993).
[2] L. D. Hicks and M. S. Dresselhaus, Physical Review B 47, 8 (1993).
[3] L. D. Hicks, T. C. Harman, X. Sun, and M. S. Dresselhaus, Physical Review B 53, R10493 (1996).
[4] G. D. Mahan and J. O. Sofo, Proceedings of the National Academy of Sciences 93, 7436 (1996).
[5] N. Nakpathomkun, H. Q. Xu, and H. Linke, Physical Review B 82 (2010).
[6] J. P. Heremans, M. S. Dresselhaus, L. E. Bell, and D. T. Morelli, Nature Nanotechnology 8, 471 (2013).
[7] A. Singha, S. D. Mahanti, and B. Muralidharan, AIP Advances 5 (2015).
[8] A. Majumdar, Science 303, 777 (2004).
[9] G. J. Snyder and E. S. Toberer, Nature Materials 7, 105 (2008).
[10] T. C. Harman, P. J. Taylor, M. P. Walsh, and B. E. LaForge, Science 297, 2229 (2002), ISSN 0036-8075.
[11] B. Poudel, Q. Hao, Y. Ma, Y. Lan, A. Minnich, B. Yu, X. Yan, D. Wang, A. Muto, D. Vashaee, et al., Science 320, 634 (2008), ISSN 0036-8075.
[12] J.-H. Bahk, Z. Bian, and A. Shakouri, Phys. Rev. B 87, 075204 (2013).
[13] M. Thesberg, H. Kosina, and N. Neophytou, Journal of Applied Physics 120, 234302 (2016).
[14] A. Singha and B. Muralidharan, Scientific Reports 7, 7879 (2017).
[15] S. Hersfield, K. A. Mutalib, and B. J. Nartowt, Phys. Rev. B 88, 085426 (2013).
[16] H. Karbaschi, J. Lovén, K. Courteaut, A. Wacker, and M. Leijnse, Physical Review B 94, 1 (2016).
[17] A. Agarwal and B. Muralidharan, Applied Physics Letters 105, 013104 (2014).
[18] B. Sothmann, R. Sánchez, A. N. Jordan, and M. Böttiker, New Journal of Physics 15 (2013).
[19] B. Sothmann, R. Sánchez, and A. N. Jordan, Nanotechnology 26, 032001 (2015).
[20] B. Muralidharan and M. Grifoni, Physical Review B 85, 1 (2012).
[21] M. Esposito, K. Lindenberg, and C. Van den Broeck, Phys. Rev. Lett. 102, 130602 (2009).
[22] M. Esposito, R. Kawai, K. Lindenberg, and C. Van den Broeck, Phys. Rev. Lett. 105, 150603 (2010).
[23] B. De and B. Muralidharan, Phys. Rev. B 94, 165416 (2016).
[24] R. S. Whitney, Physical Review Letters 112, 1 (2014).
[25] R. S. Whitney, Physical Review B 91, 1 (2015).
[26] C. H. Schiegg, M. Dzierzawa, and U. Eckern, Journal of Physics: Condensed Matter 29, 085303 (2017).
[27] P. Priyadarshi, A. Sharma, S. Mukherjee, and B. Muralidharan, Journal of Physics D: Applied Physics 51, 185301 (2018).
[28] D. A. Broïdo and T. L. Reinecke, Physical Review B 51, 13797 (1995).
[29] H. H. Tung and C. P. Lee, IEEE Journal of Quantum Electronics 32, 507 (1996).
[30] S. Mukherjee, P. Priyadarshi, A. Sharma, and B. Muralidharan, IEEE Transactions on Electron Devices 65, 1896 (2018), ISSN 0018-9383.
[31] C. Facher, C. Rauch, G. Strasser, E. Gornik, F. Elsholz, A. Wacker, G. Kießlich, and E. Schöll, Applied Physics Letters 79, 1486 (2001).
[32] S. Mukherjee and B. Muralidharan, Integrated Ferroelectrics 194 (2018).
[33] J. Martorell, D. W. L. Sprung, and G. V. Morozov, Physical Review B 69, 115309 (2004), ISSN 01631829.
[34] G. V. Morozov, D. W. L. Sprung, and J. Martorell, J. Phys. D 335, 3052 (2002).
[35] S. Datta, Quantum Transport: Atom to Transistor (Cambridge University Press, 2005).
[36] S. Datta, Lessons from Nanoelectronics: A New Perspective on Transport, Lecture notes series (World Scientific Publishing Company, 2012).