The Phonovoltaic Cell

Abstract **– A new energy conversion device, the phonovoltaic cell, is proposed. In this cell, a non-equilibrium (hot) population of optical phonons more energetic than the bandgap produces electron-hole pairs in a *p-n* junction, which separates them to produce power. That is, it harvests optical phonons like a photovoltaic harvests photons. To date, the function of the phonovoltaic cell has been modeled [2] and suitable materials for the device have been investigated and designed [3,4]. Results suggest that the phonovoltaic cell can harvest optical phonons ("heat") at high fractions of the Carnot limit and with double to triple the efficiency of a thermoelectric generator [4].**

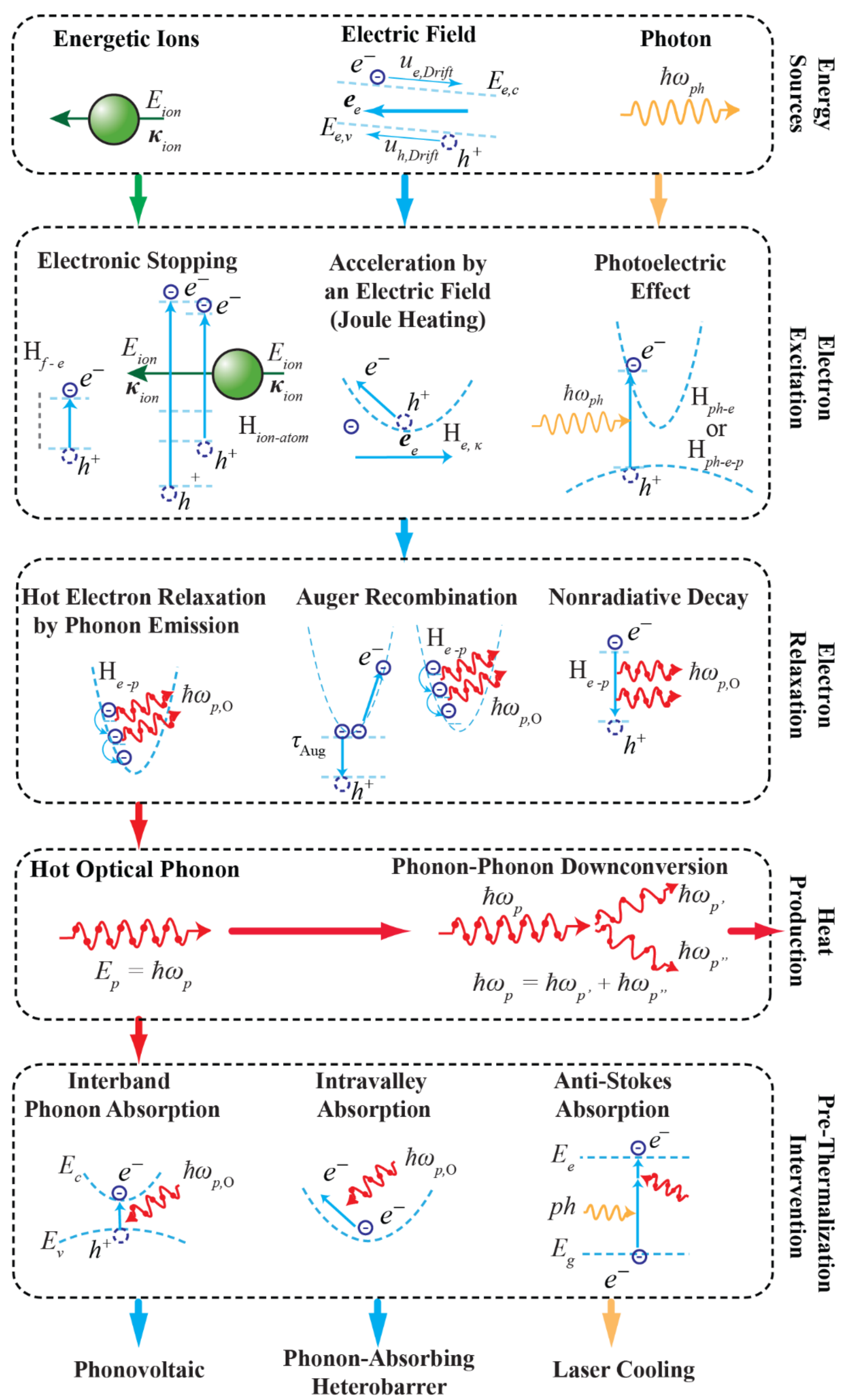

Figure 1. Typical Energy pathways

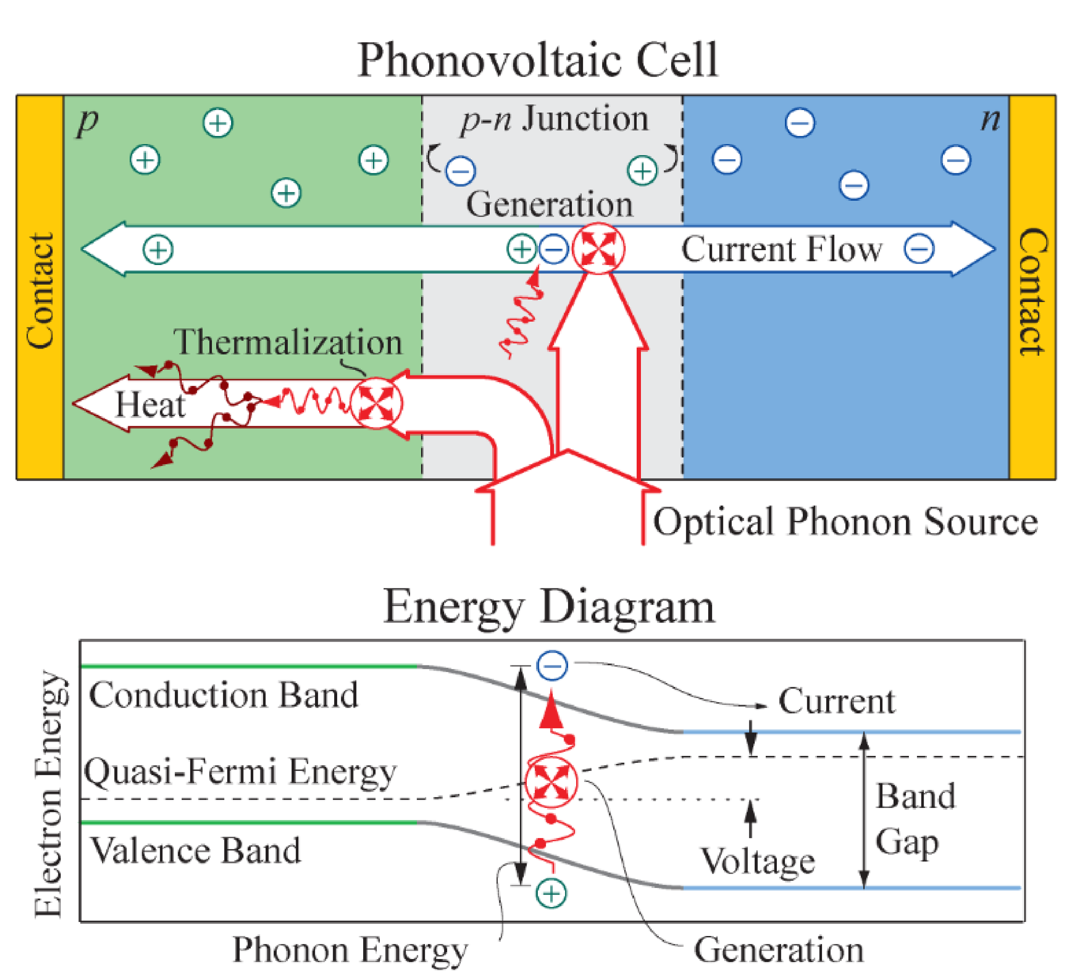

Figure 2. The phonovoltaic cell and its energy diagram

Motivation - Figure 1

Optical phonons are an intermediate product of energy excitations on the path towards thermalization and heat production. The hot, or excited, population of optical phonons which result from an energy excitation like a laser or electric field has substantially less entropy than heat (a broad collection of acoustic phonons). Thus, we should be able to harvest them with much greater efficiency than we can harvest heat.

Challenges

Unfortunately, optical phonons thermalize quickly – typically within picoseconds and over tens of nanometers. This has largely prevented the invention of a successful heat harvesting scheme. Laser cooling and optical refrigeration, which utilizes anti-stokes processes during phonon assisted photon absorption, is one such attempt. However, the process typically requires extremely low temperatures. Phonon absorbing heterobarriers are another example. However, the process requires extremely low currents to function, limiting its applicability. (See the research page for a brief summary of these topics.)

Additionally, optical phonon energies are limited. In typical materials, the maximum optical phonon energy is limited to below 50 meV, only twice the thermal energy (k_BT) at room temperature. While more exotic materials like graphene have optical phonon modes which reach energies of 200 meV, this is still less than $10k_BT$. This can pose a substantial obstacle to their harvest at room temperature. Indeed, it is one of the major challenges facing the phonovoltaic cell.

The Phonovoltaic Cell – Figure 2

Despite this challenge, the phonovoltaic cell depicted in Fig. 2 is the most promising device we have invented or investigated yet. This energy conversion cell harvests optical phonons much like a photovoltaic harvests photons; thus, the name: phonon-voltaic becomes phonovoltaic.

To be more precise, in the phonovoltaic a non-equilibrium (hot) population of optical phonons more energetic than the bandgap produces electron-hole pairs in a *p-n* junction, which separates them to produce power. The efficiency (η_{pV}) of this process and material figure of merit (Z_{pV}) which determines it are

$$Z_{pV} = \gamma^*_{e\text{-}p}\,\Delta E^*_{e,g}$$
$$\eta_{pV} = \eta_C\, Z_{pV}\, F_F^*,$$

where $\gamma^*_{e\text{-}p}$ and $\Delta E^*_{e,g}$ quantify the fraction of optical phonons which relax by producing heat rather than electrons and the fraction of the optical phonon energy which is preserved by the bandgap and F_F^* is the adjusted fill-factor of the *p-n* junction [2].

Material Requirements - Figure 3

In the photovoltaic, incoming photons only produce power when they are more energetic than the energy gap between the valence and conduction states (the bandgap, $E_{e,g}$). Similarly, the optical phonons in a material must be more energetic than the bandgap in order for them to produce power, rather than heat. Moreover, they must be much more energetic than the thermal energy, otherwise electrons in the conduction states will block generation due to the Pauli exclusion principle [4]. Finally, a good phonovoltaic material requires that its optical phonon modes couple to its electrons more strongly they couple with other phonon modes. (The latter coupling drives thermalization and heat production.)

In summary, we require at minimum that a phonovoltaic material has

$$E_{p,O} \geq E_{e,g} >> k_BT,$$

where $E_{p,O}$ is the optical phonon energy. Figure 3 shows that this condition is rarely met. In the vast majority of materials, the optical phonon energy is comparable to the thermal energy and proportional to but much less than the bandgap. Thus, *the vast majority of materials are not suited for use in a phonovoltaic cell.* However, graphene is an exception – it has no bandgap and 200 meV optical phonon modes – which has proven to be very suitable.

Tuned Graphene – Figure 4

The bandgap in graphene may be opened to enable its use in electronic devices like the phonovoltaic cell. Multiple methods have been suggested to do this, including the application of electric fields or the chemical doping of pure graphene. In general, these methods work by altering the

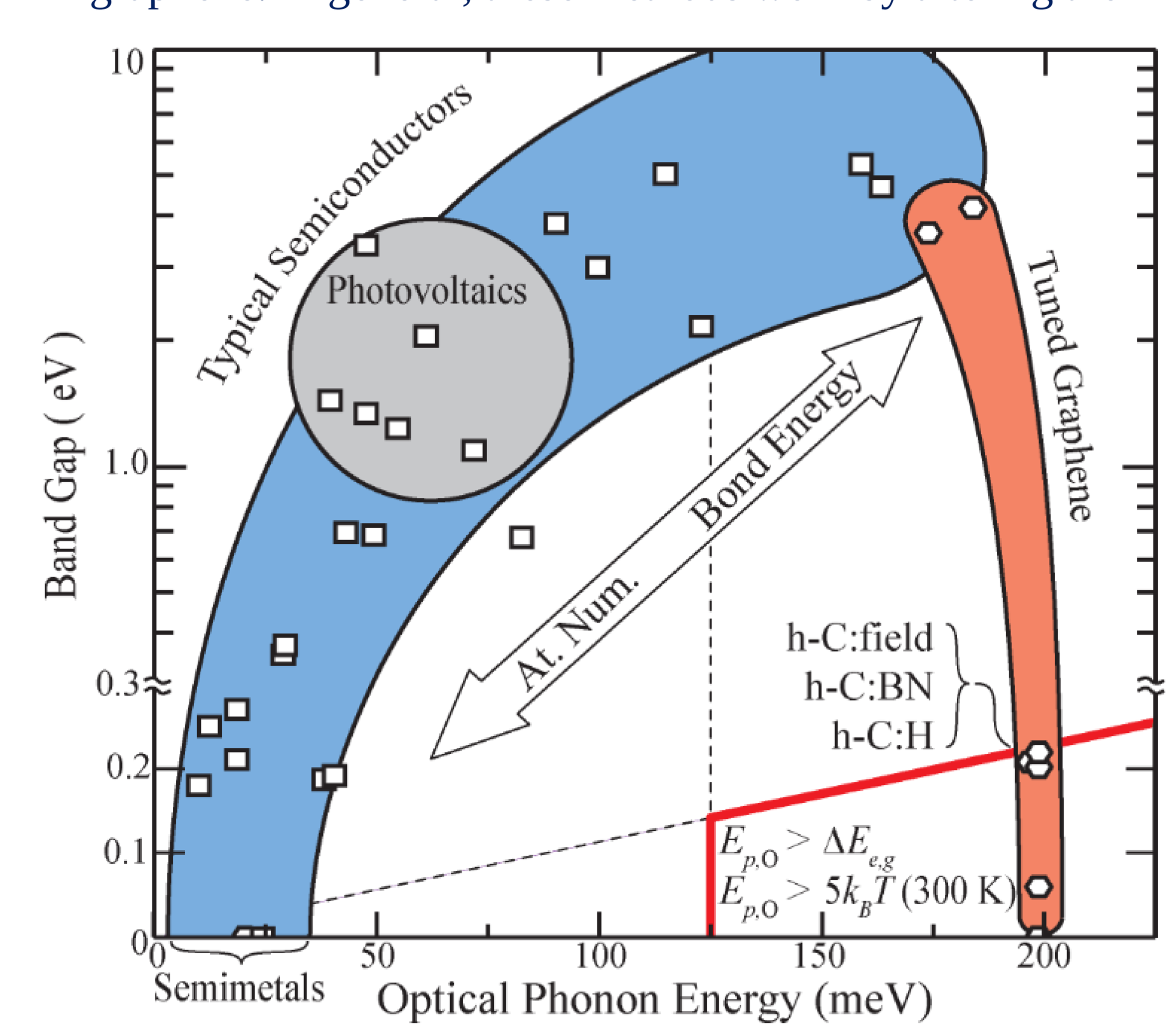

Figure 3. Material bandgap vs. optical phonon energy

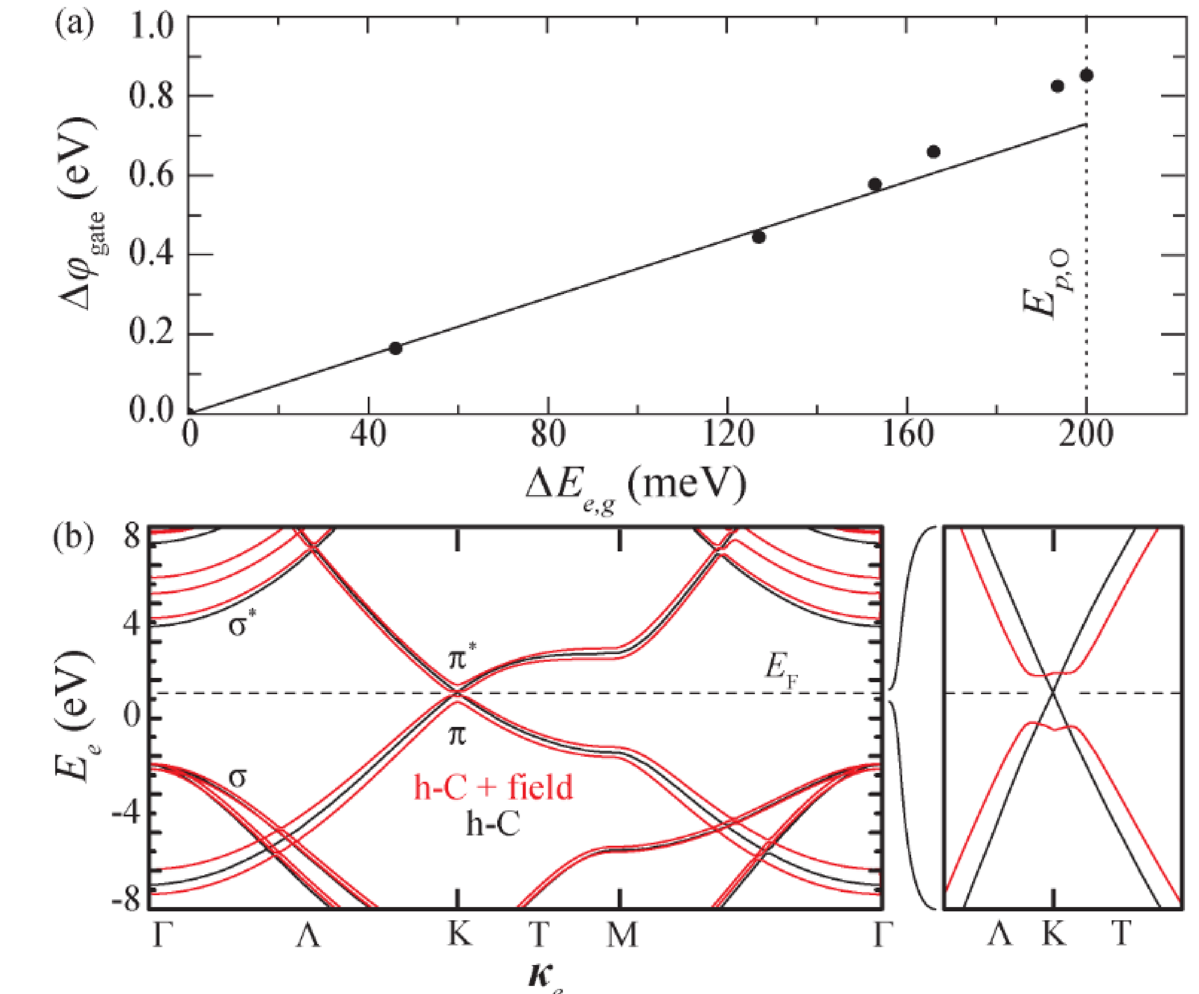

Figure 4. Bandgap and bandstructure of bilayer graphene

symmetry (the two carbon atoms in the graphene unit cell are identical) or hybridization (the sp^2 hybridization leaves an electron free per carbon atom) of graphene.

In the first material investigations, we have posited that the latter method destroys the strong electron-phonon coupling in graphene [3] while the former method preserves it [4]. Thus, by tuning the asymmetry of graphene, e.g., by doping the structure with boron-nitride [4] or by applying a cross-plane electric field to bilayer-graphene (Figure 4), one can open and tune the bandgap of graphene to its optical phonon energy while maintaining its desirable phonon kinetics. Therefore, tuned graphene materials like graphene:BN and bilayer-graphene reach a substantial figure of merit (0.65 and 0.92, respectively).

Efficiency – Figure 5

The efficiency enabled by the phonovoltaic materials investigated is presented in Figure 5. It shows that the efficiency of a phonovoltaic cell can greatly outperform a typical thermoelectric generator. Indeed, a bilayer-graphene phonovoltaic may approach conventional heat harvesting efficiencies on the nano- rather than decameter scale.

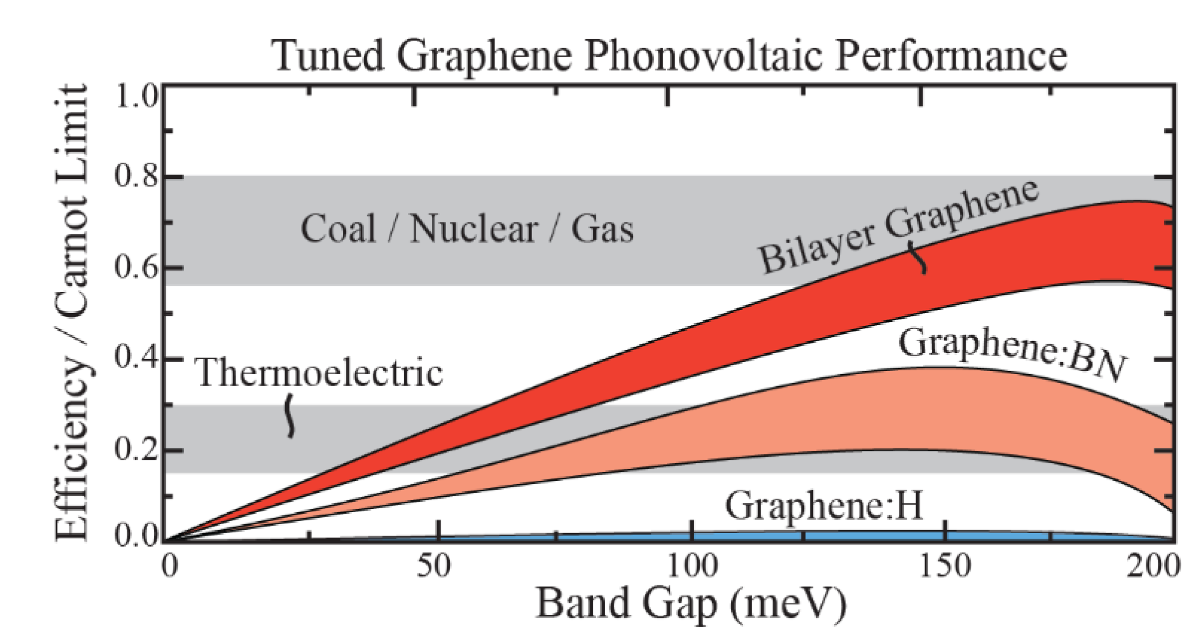

Figure 5. Efficiency vs bandgap for tuned graphene

[1] en.wikipedia.org/wiki/Phonovoltaic [2] C. Melnick and M. Kaviany, *Phys. Rev. B*, **93**, 094302 (2016) [3] C. Melnick and M. Kaviany, *Phys. Rev. B*, **93**, 125203 (2016) [4] C. Melnick and M. Kaviany, *Phys. Rev. B*, **94**, 245412 (2016)