

# NEAR-FIELD RADIATIVE TRANSFER

*For Energy Harvesting.... & Diagnostic+Manufacturing*

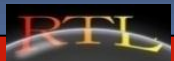
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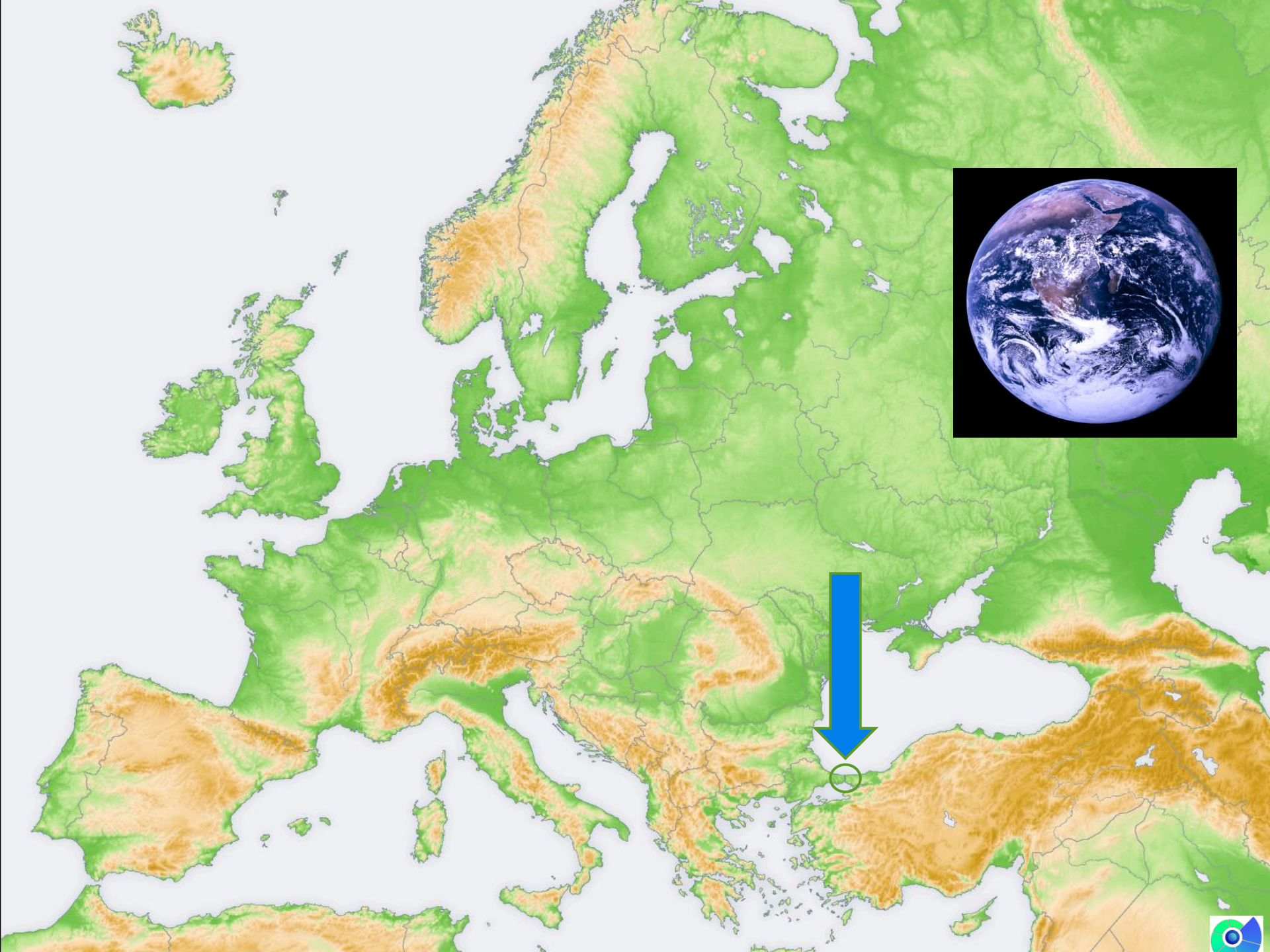


MSEWS<sub>4</sub>: Energy Conservation and Waste Heat Recovery  
November 21, 2013  
IPAM, UCLA, LA, CA, USA



# OUTLINE OF PRESENTATION

- **The Big Picture**
- **Overview of Far and Near-Field Radiative Transfer**
- **Length Scales for Nano-regimes**
- **Near Field Radiation**
- **Near Field Radiation for Thermophotovoltaics (TPV) Applications**
- **Analytical Analysis**
- **Computational Analysis**
- **Conclusions**



We are here...



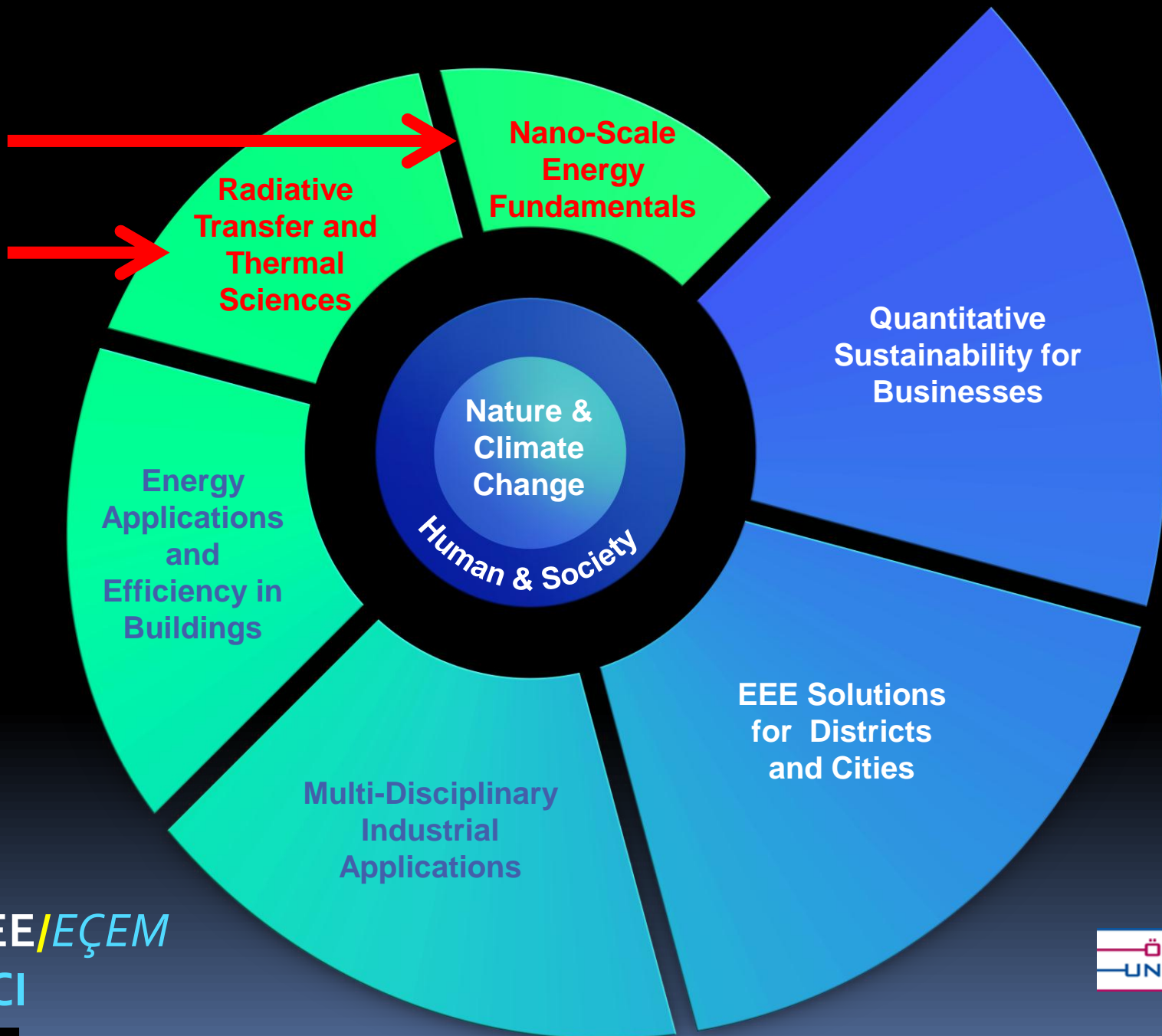
UK



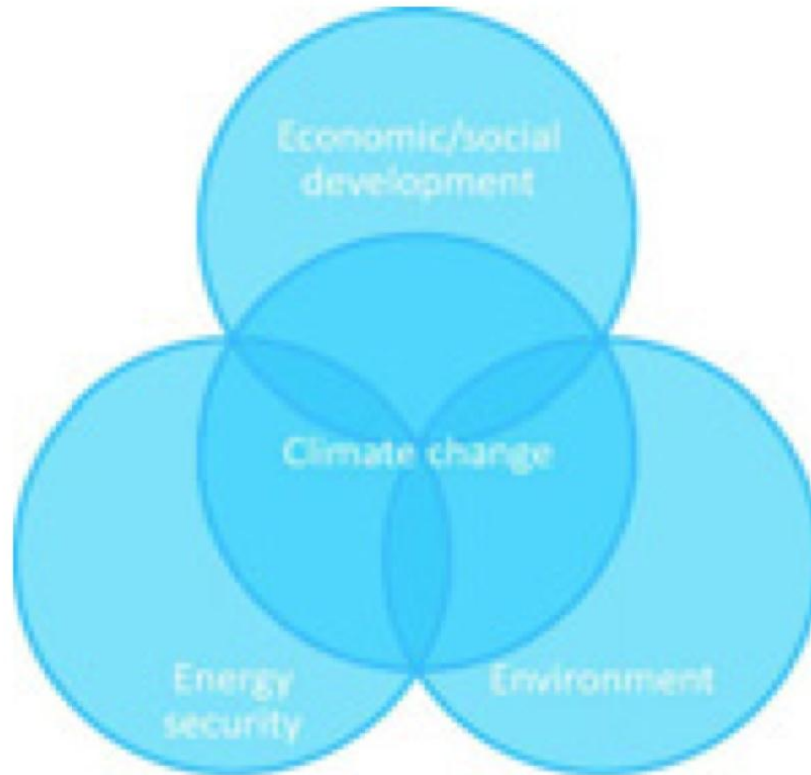
CEEE/EÇEM

ÖZYEĞİN  
UNIVERSITY

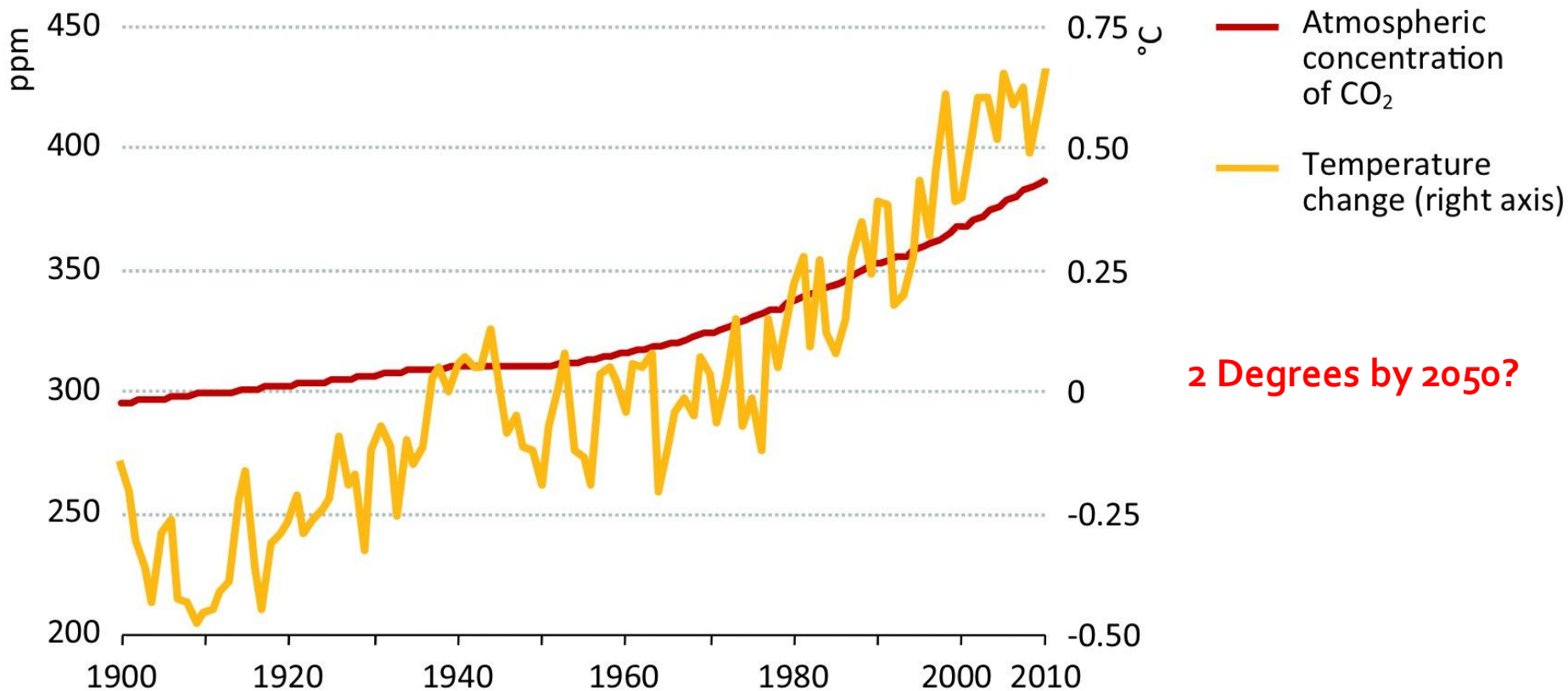




## Linkages between climate change and other major policies



# CLIMATE CHANGE? (IEA 2013)



Note: The temperature refers to the NASA Global Land-Ocean Temperature Index in degrees Celsius, base period: 1951-1980. The resulting temperature change is lower than the one compared with pre-industrial levels.

Sources: Temperature data are from NASA (2013); CO<sub>2</sub> concentration data from NOAA Earth System Research Laboratory.

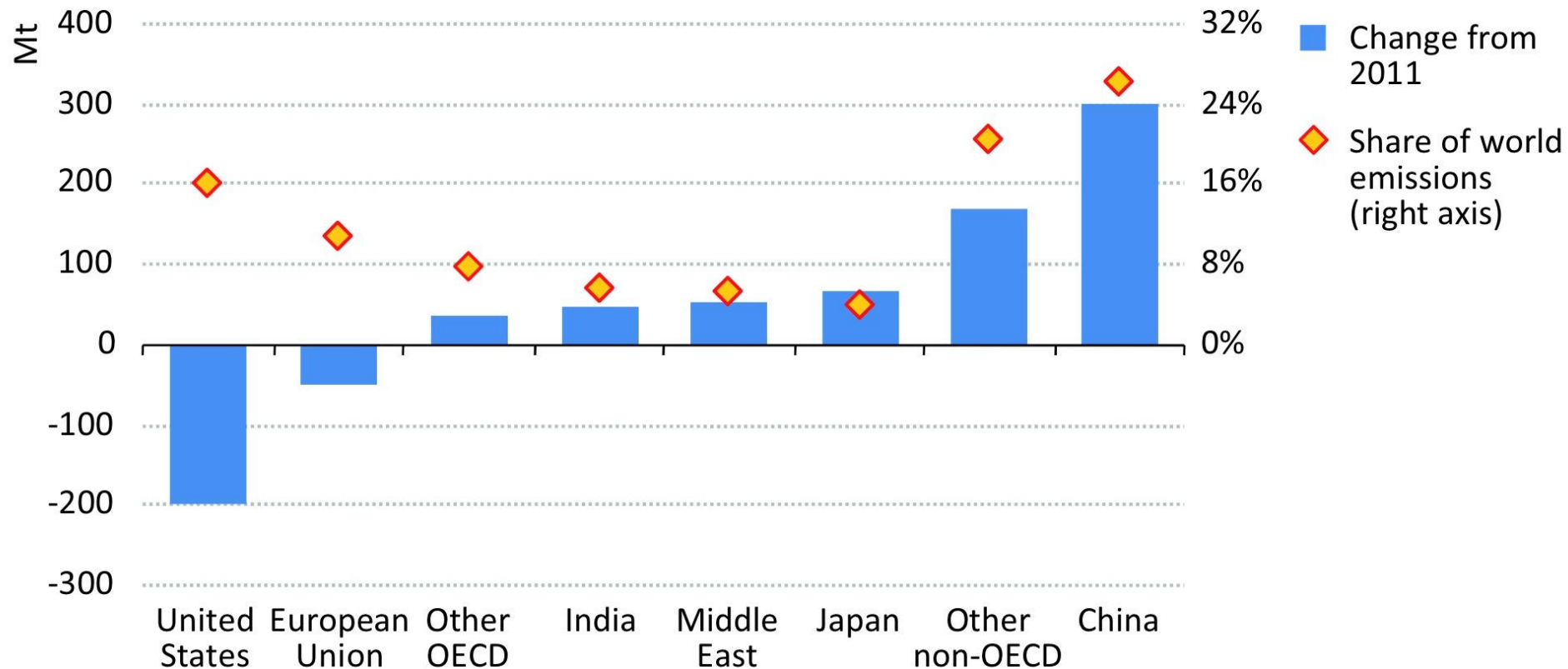
**EVERY TON OF CO<sub>2</sub> RELEASED TO THE ATMOSPHERE**

**...CORRESPONDS TO WASTED ENERGY ENDING UP  
SOMEWHERE!**

**MINIMIZATION OF ENERGY USE HELPS DECREASING  
EMISSIONS OF CO<sub>2</sub>.**

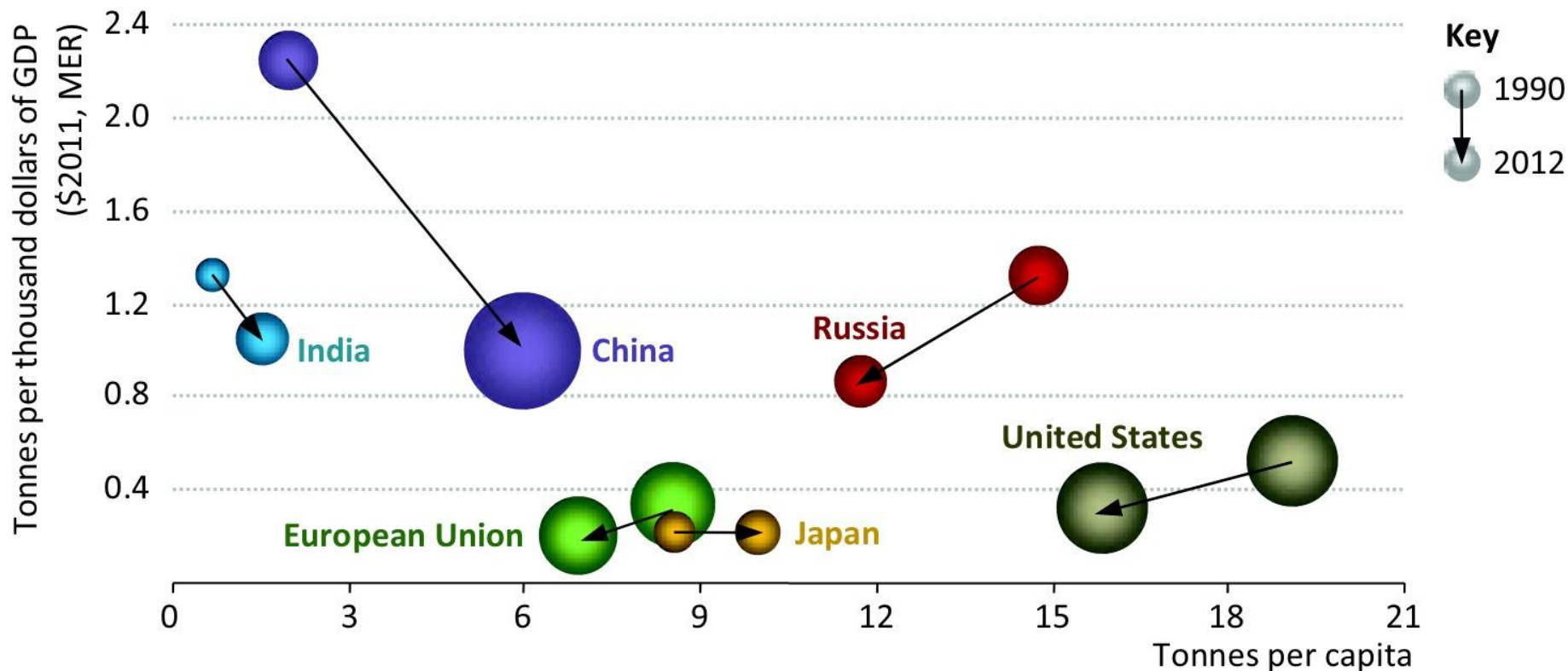
# ONE-YEAR CO<sub>2</sub> EMISSION TRENDS CHANGE (IEA 2013)

**Figure 1.8** ▶ CO<sub>2</sub> emissions trends in 2012



# ENERGY RELATED CO<sub>2</sub> EMISSIONS (IEA 2013)

**Figure 1.14** ▶ Energy-related CO<sub>2</sub> emissions per capita and CO<sub>2</sub> intensity in selected regions



Notes: Bubble area indicates total annual energy-related CO<sub>2</sub> emissions in that region. MER = market exchange rate.

**BIG PICTURE:**

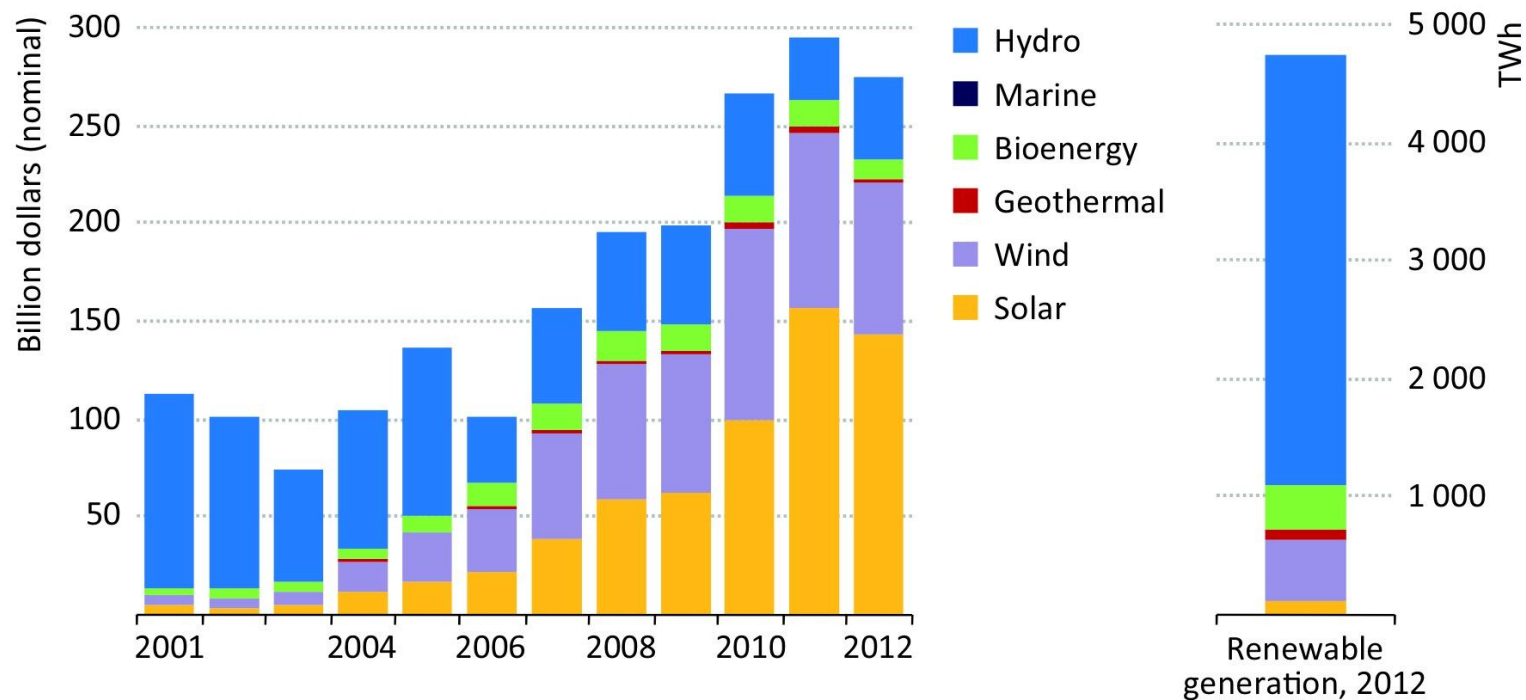
**WORLD ENERGY USE IS ABOUT 15 TW.**

**CO<sub>2</sub> EMISSIONS ARE RELATED TO FOSSIL ENERGY USE.**

**ONLY A FRACTION OF ENERGY GENERATED IS FROM  
RENEWABLES.**

# WORLD RENEWABLE ENERGY USE (IEA 2013)

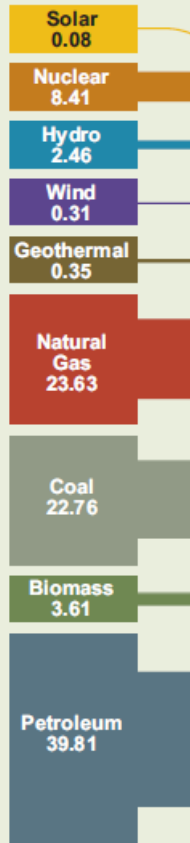
**Figure 1.5** ▶ World renewables-based power sector investment by type and total generation



Note: TWh = terawatt-hours.

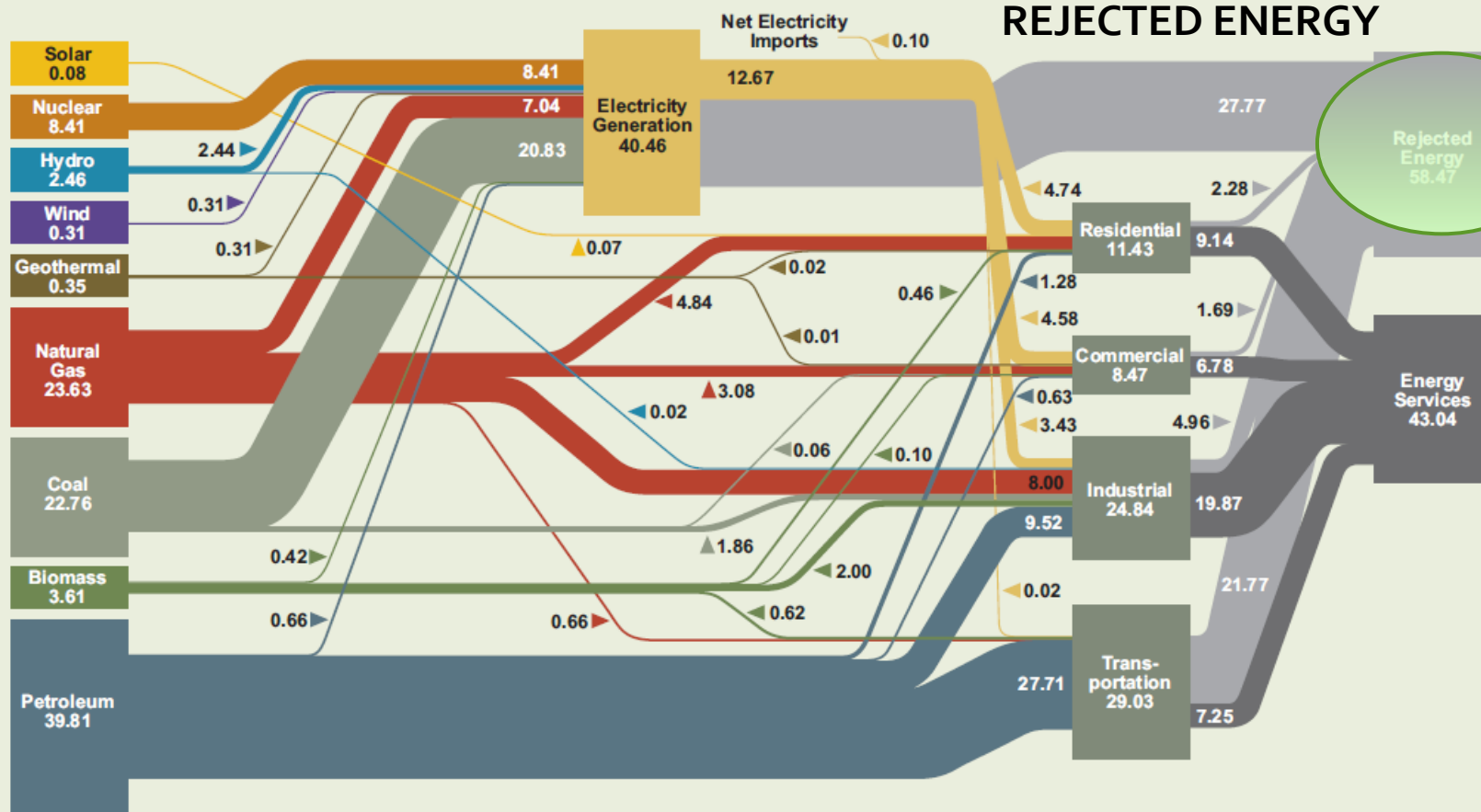
Sources: BNEF (2013); Frankfurt School UNEP Collaborating Centre and Bloomberg New Energy Finance (2012); and IEA data and analysis.

# ENERGY MODALITIES



Energy Production Modalities

# ENERGY MODALITIES

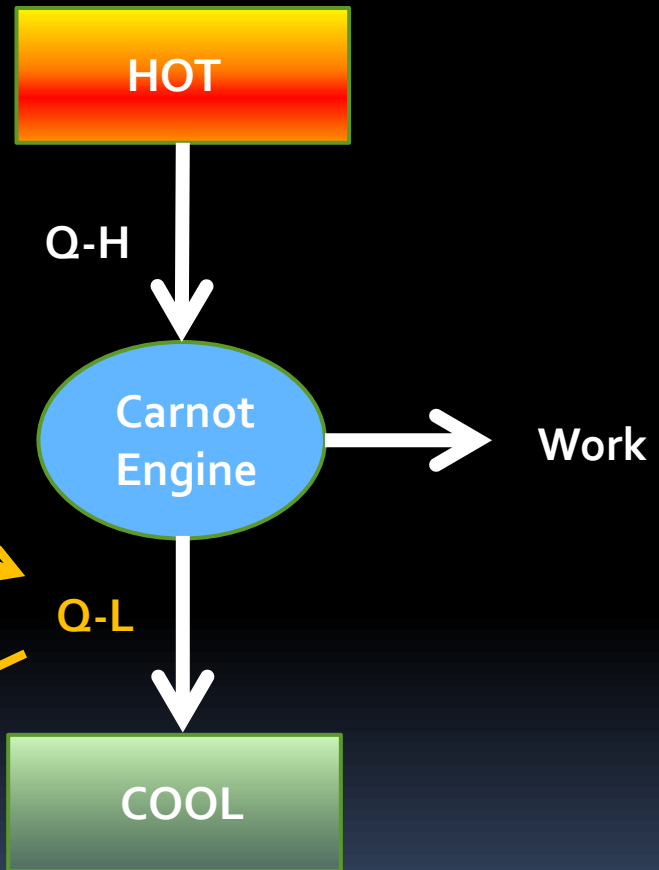


Wasted Energy should be used somehow!

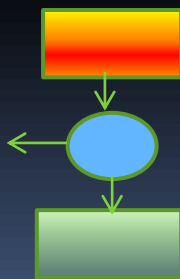
- Energy Generation
- Energy Conservation/Efficiency
- Energy Harvesting

# ENERGY HARVESTING

Energy Harvesting is to recover wasted energy from all sources to be used as auxiliary energy source, for electricity generation or for storage.



What to do with Q-L?



Carnot Efficiency:

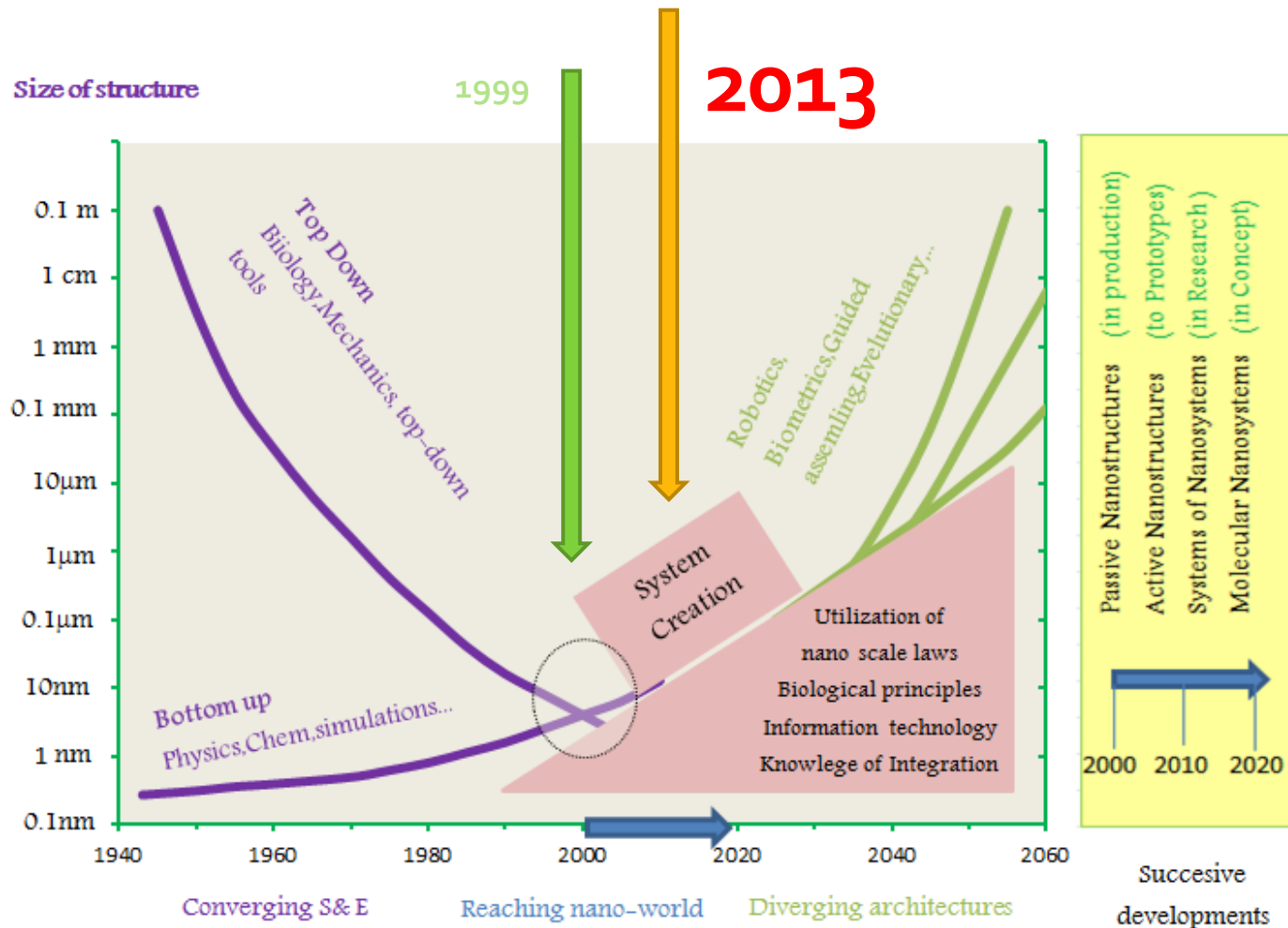
$$\eta = W/Q$$

# CONVERGENCE

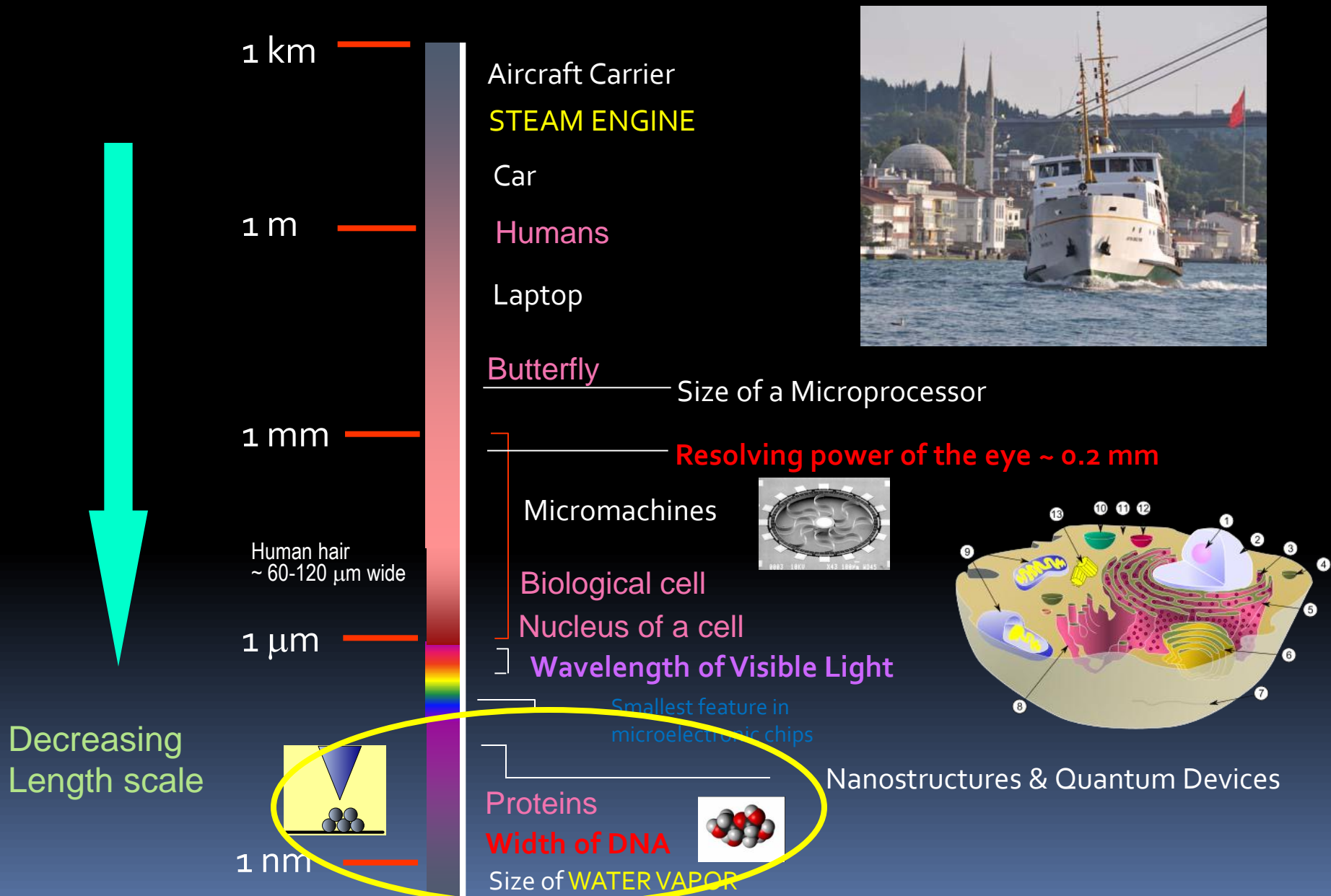
Solve Energy Challenge *via*

Advanced Engineering on Fundamental Physics

# INSPIRATION: REACHING NANO-WORLD ... From 2005 ROCO!

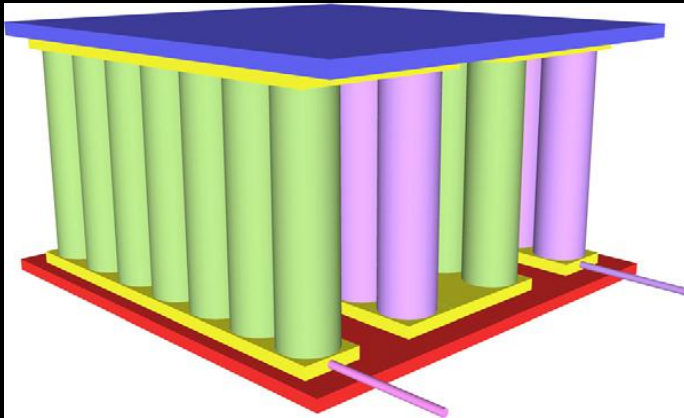


# PERSPECTIVE ON LENGTH SCALES



# HOW TO RECOVER WASTE ENERGY?

## Thermoelectric Devices (conduction/phonon based)



Nondimensional figure of merit:

$$ZT = \sigma S^2 T / \kappa$$

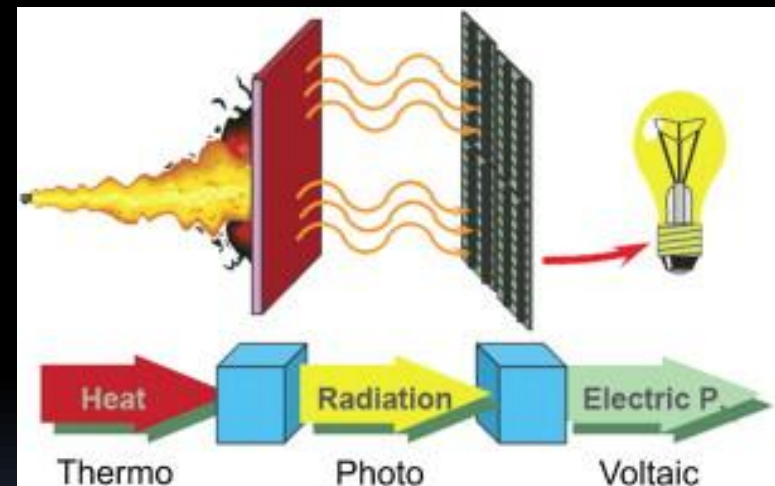
$\sigma$  : the electrical conductivity

$S$  : the Seebeck coefficient

$T$  : the temperature

$\kappa$  : the thermal conductivity

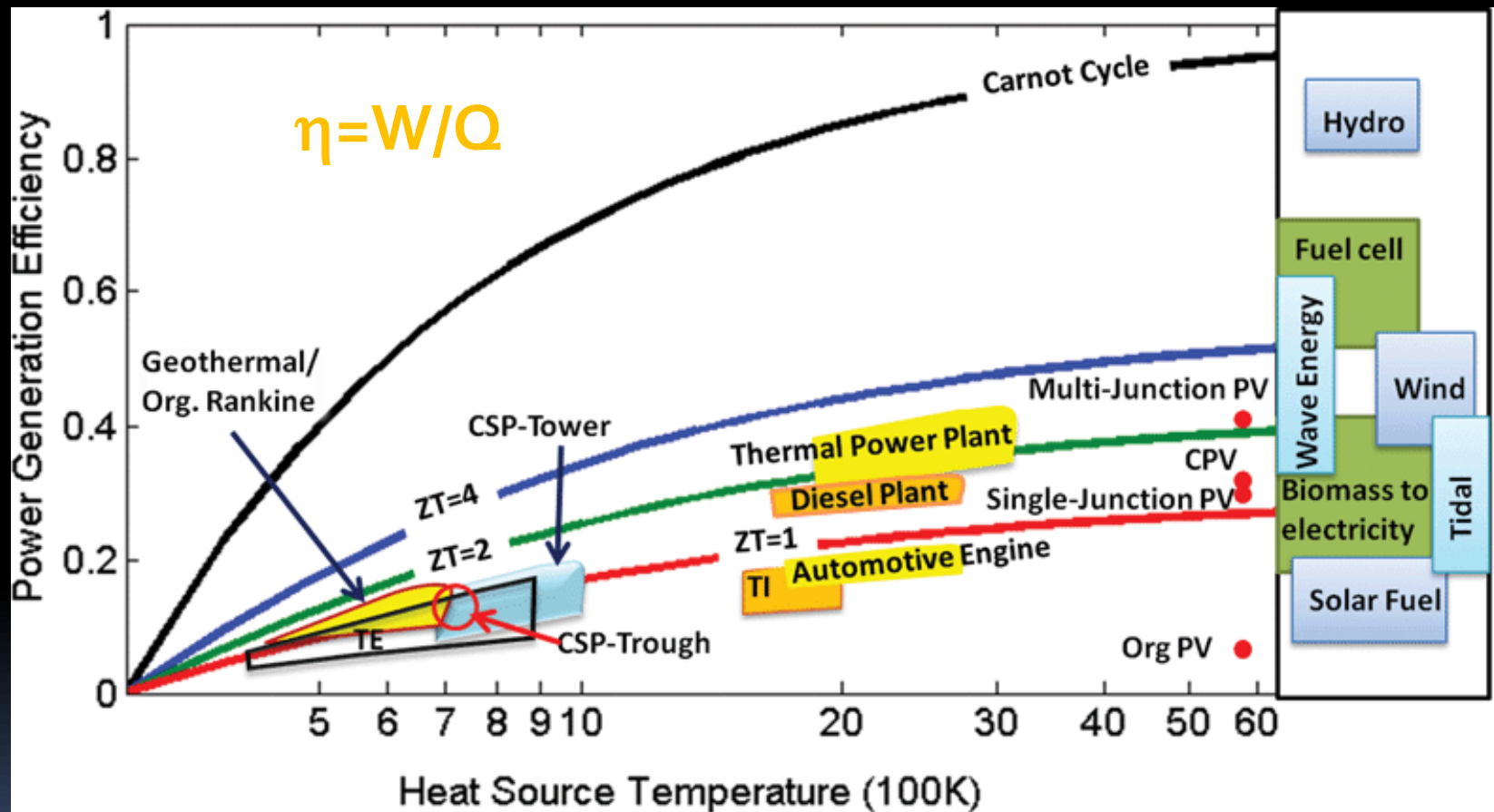
## Thermophotovoltaic Devices (Radiation/near-field radiation transfer based)



## Optical heat engine!

(Figs from web sources!)

# POWER GENERATION EFFICIENCY



Zebarjadi, et al. *Energy Environ. Sci.*, 2012, 5, 5147-5162.

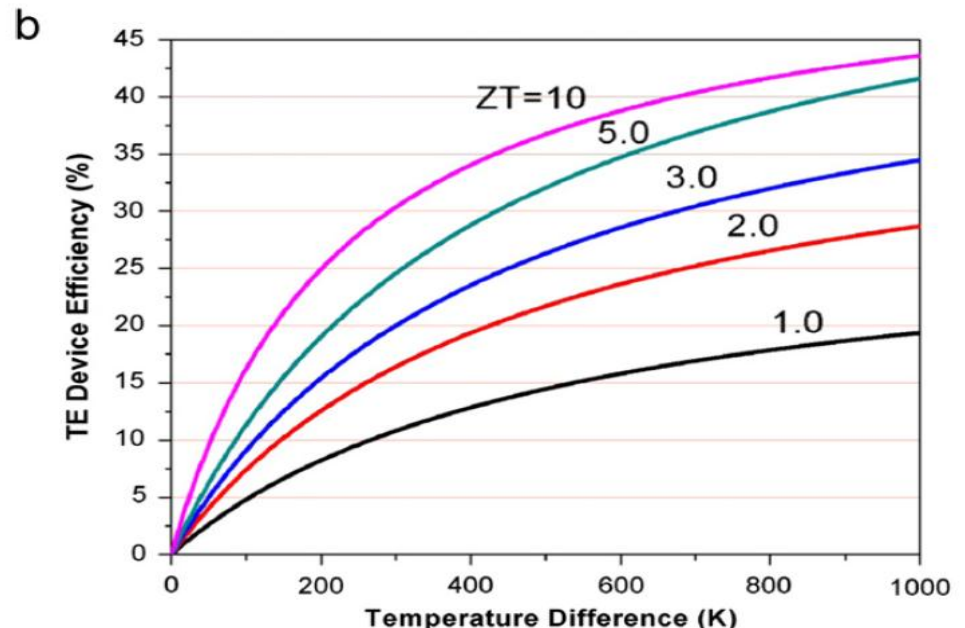
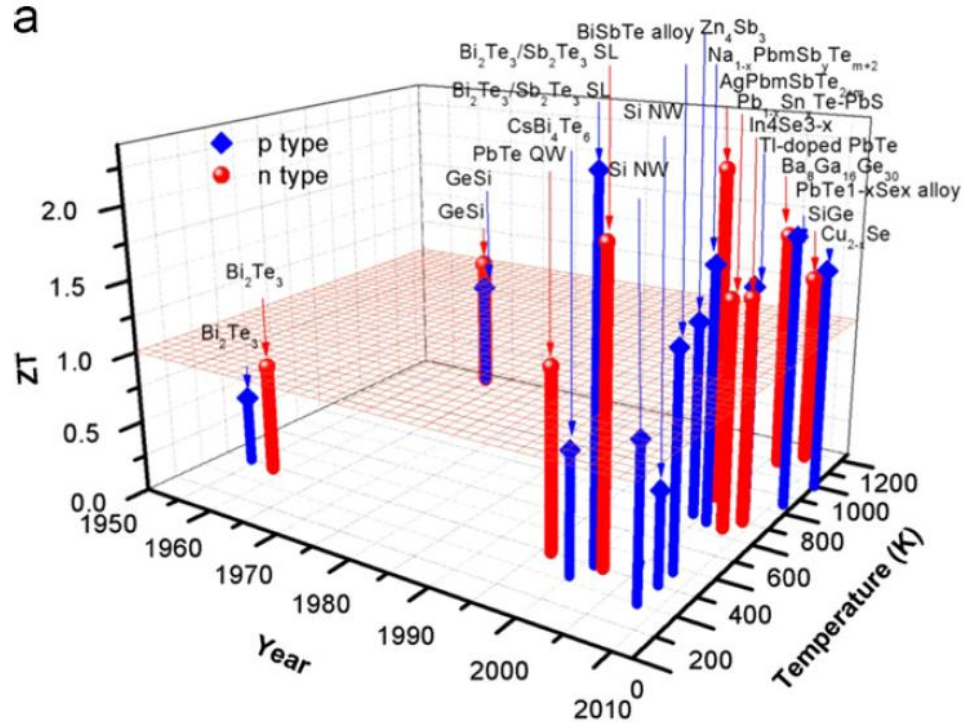
# THERMOELECTRIC DEVICES

Thermoelectric power generators are solid state devices which can directly convert heat into electricity.

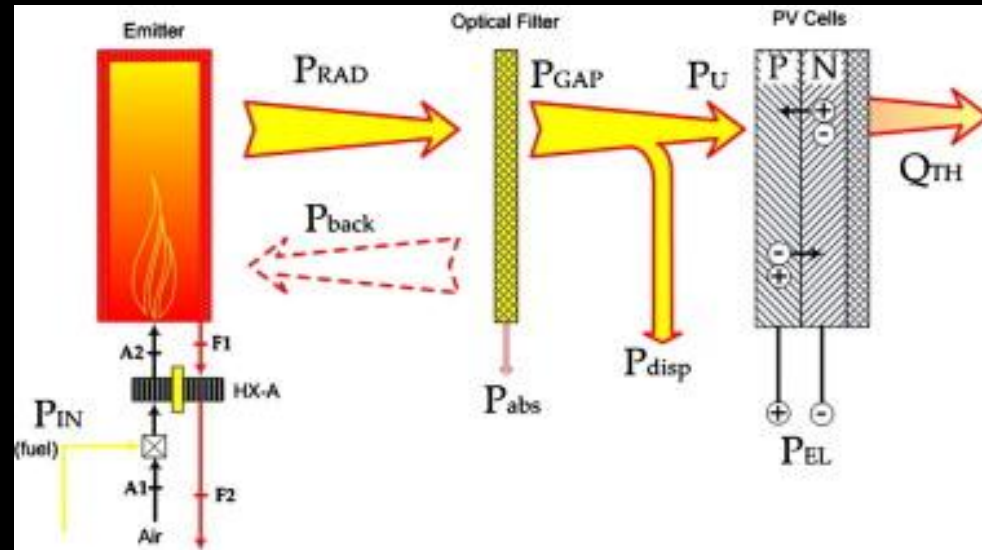
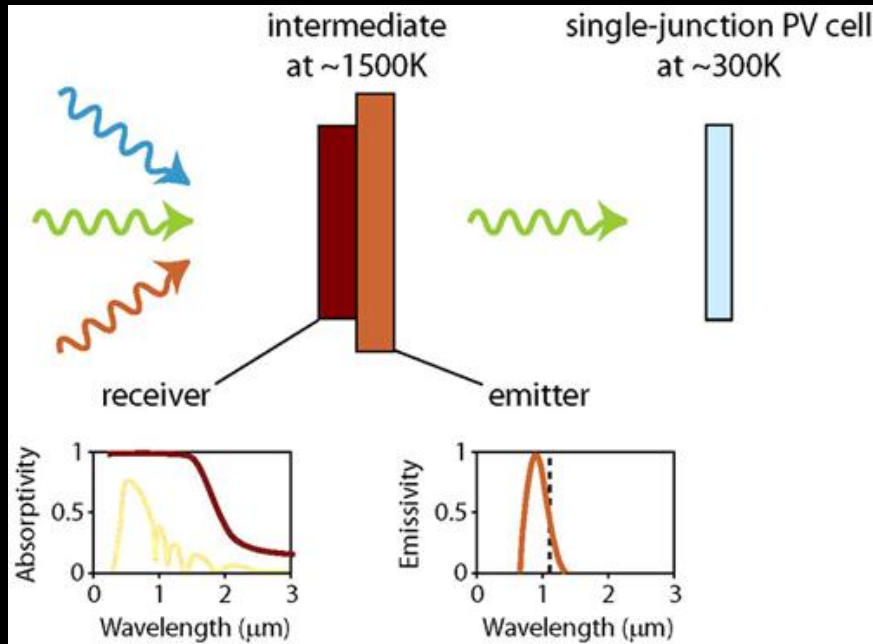
The device efficiency depends on the choice of material, configuration, and contacts.

It requires new materials, dopants, and nanostructured geometries.

**MATERIAL PROBLEM!**



# TPV CELL



Schematic of the thermophotovoltaic cell proposed by Fan group. The idealized absorption spectrum (solar spectrum in yellow) and emission spectrum (the dotted line: PV cell bandgap energy level) are shown.

[http://gcep.stanford.edu/research/factsheets/ultrahigh\\_thermosolar.html](http://gcep.stanford.edu/research/factsheets/ultrahigh_thermosolar.html)

Schematic of the industrial thermophotovoltaic cell.

# THERMOPHOTOVOLTAIC DEVICES

## Potential Applications of TPVs:

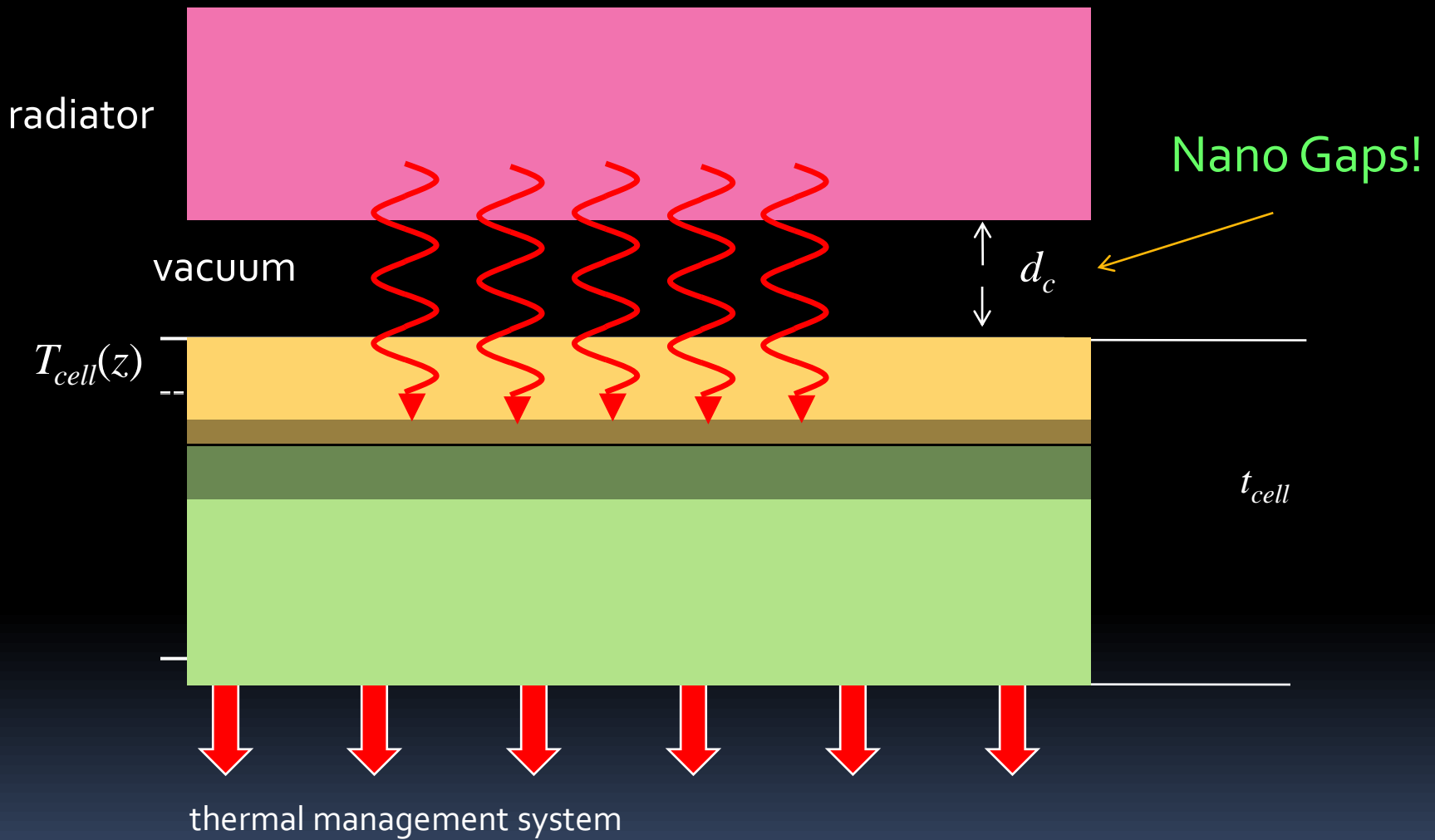
- Power sources for Micro-electromechanical devices (MEMS).
- Energy sources in transportation.
- Co-generation of electricity and heat.
- Remote electricity generators.
- Aerospace and military power suppliers.
- And..

Waste-Energy harvesting purposes.

# THERMOPHOTOVOLTAIC DEVICES

- How can we improve the efficiency of TPV Devices?
  - Materials?
  - Design and Geometry?

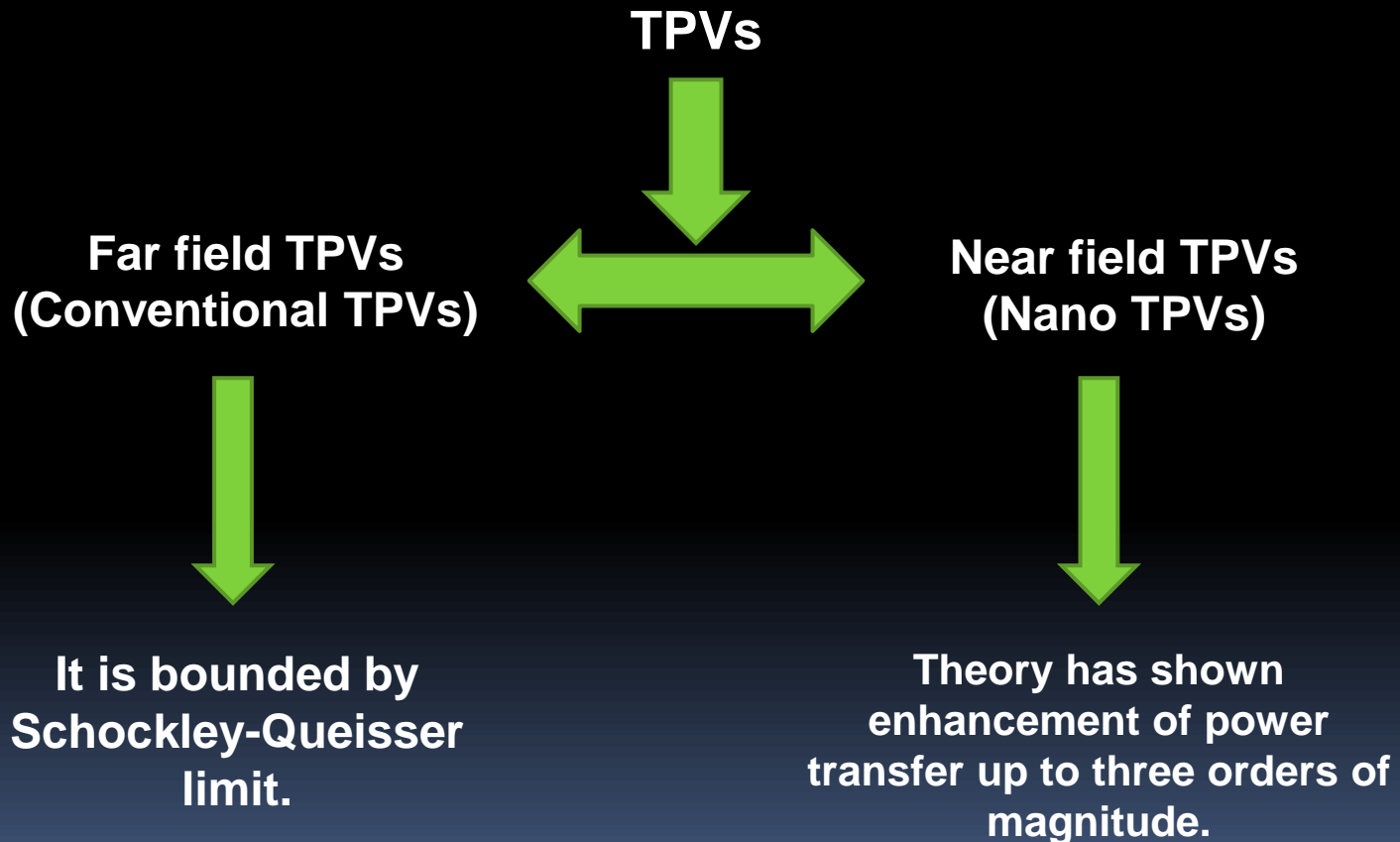
# TPV? Nano-TPV?



OBJECTIVE: RADIATE SELECTIVELY TO THE CELL ...

# THERMOPHOTOVOLTAIC DEVICES

**Thermophotovoltaics (TPVs):** energy-conversion systems generating an electric current from the thermal photons radiated by a hot body.



DOI: 10.1038/srep01383

# THERMOPHOTOVOLTAIC DEVICES

## Far-field PV

Ability to control plasmon damping **X**

High power density **X**

ability to operate in the intermediate (600–1200K) emitter temperature range **X**

Emitter plasmon frequencies optimally match to the bandgap **X**

## Near-field PV

Ability to control plasmon damping **✓**

High power density **✓**

Ability to operate in the intermediate (600–1200K) emitter temperature range **✓**

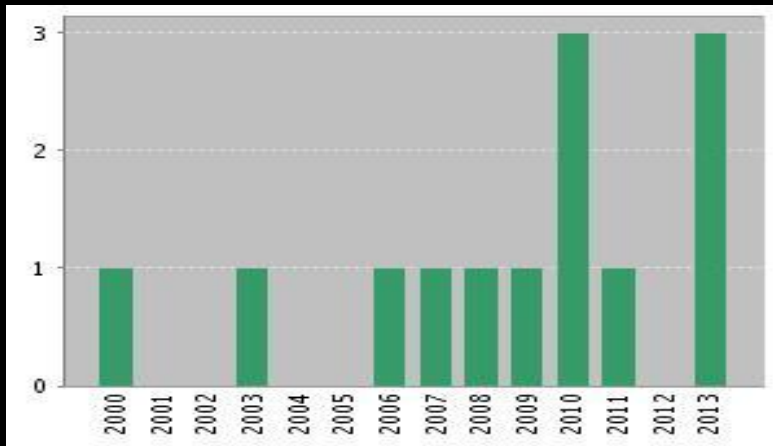
Emitter plasmon frequencies optimally matches to the bandgap **✓**

Ilic, Ognjen et al. "Overcoming the Black Body Limit in Plasmonic and Graphene Near-field Thermophotovoltaic Systems." *Optics Express* 20.53 (2012): A366. © 2012 OSA

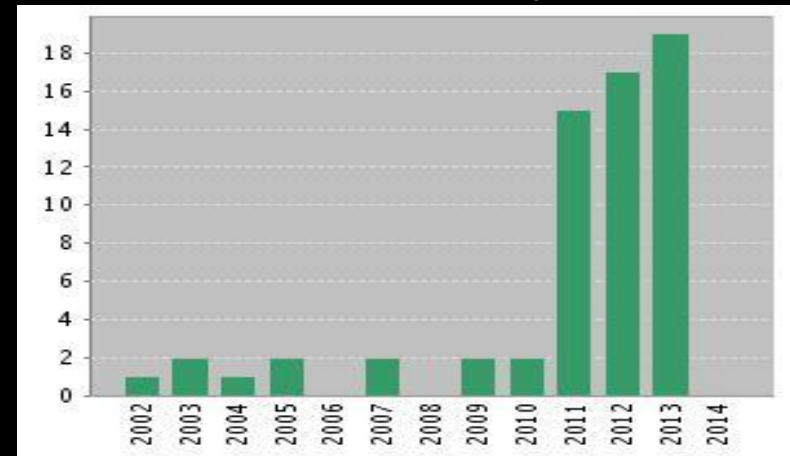
# FAR AND NEAR FIELD RADIATIVE TRANSFER

# Near- Field Publications Statistics

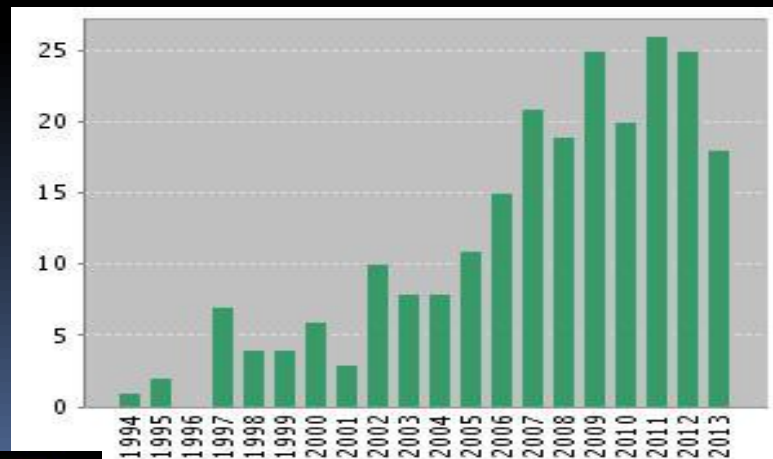
Nano Thermophotovoltaic  
Published items in each year



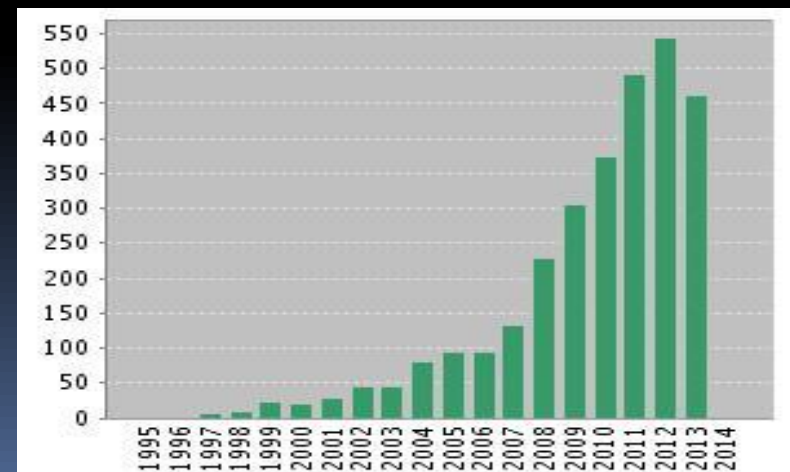
Nano Thermophotovoltaic  
Citation in each year



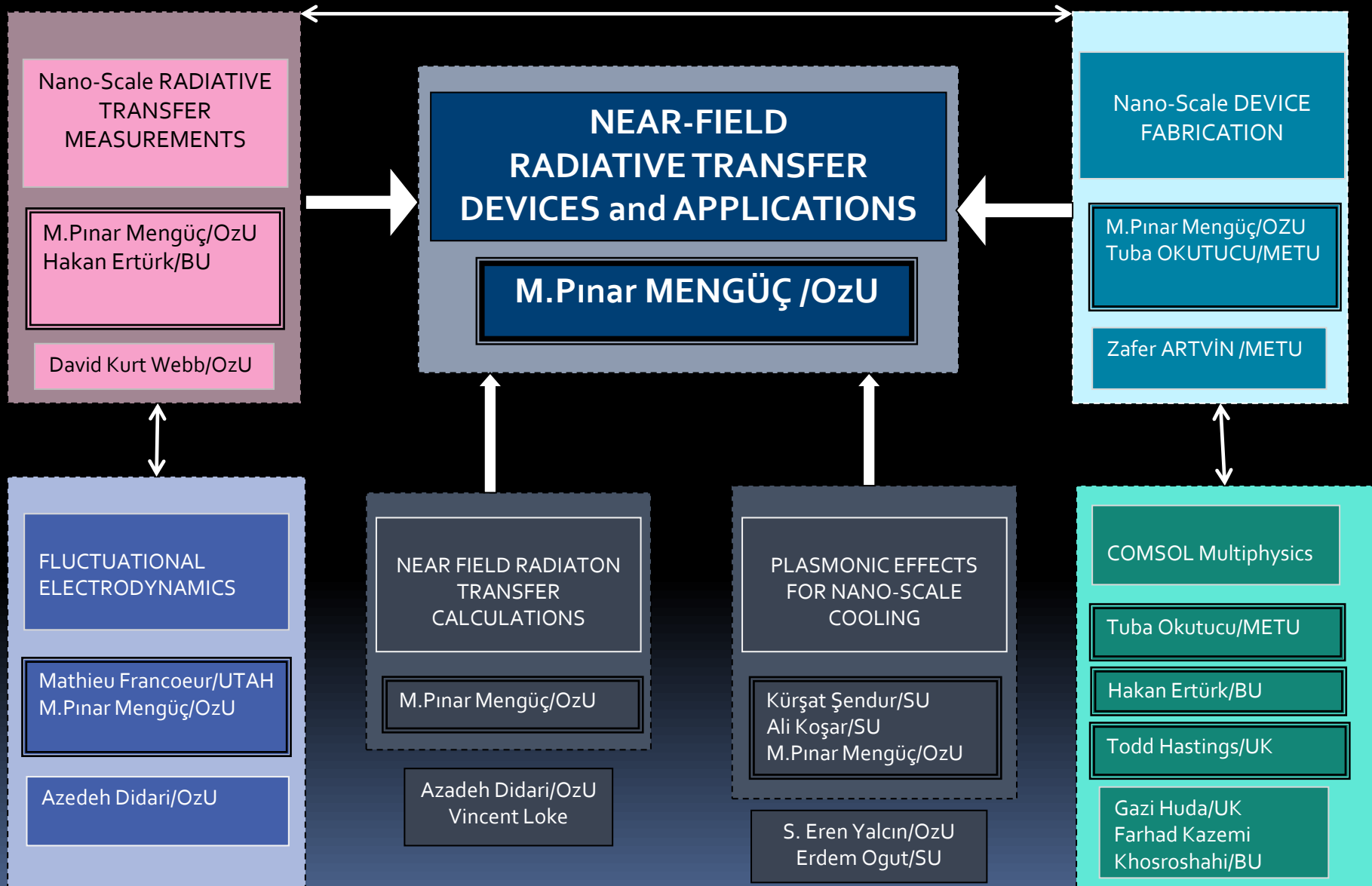
Near-field thermal radiation  
Published items in each year



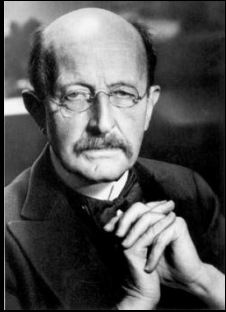
Near-field thermal radiation  
Citation in each year



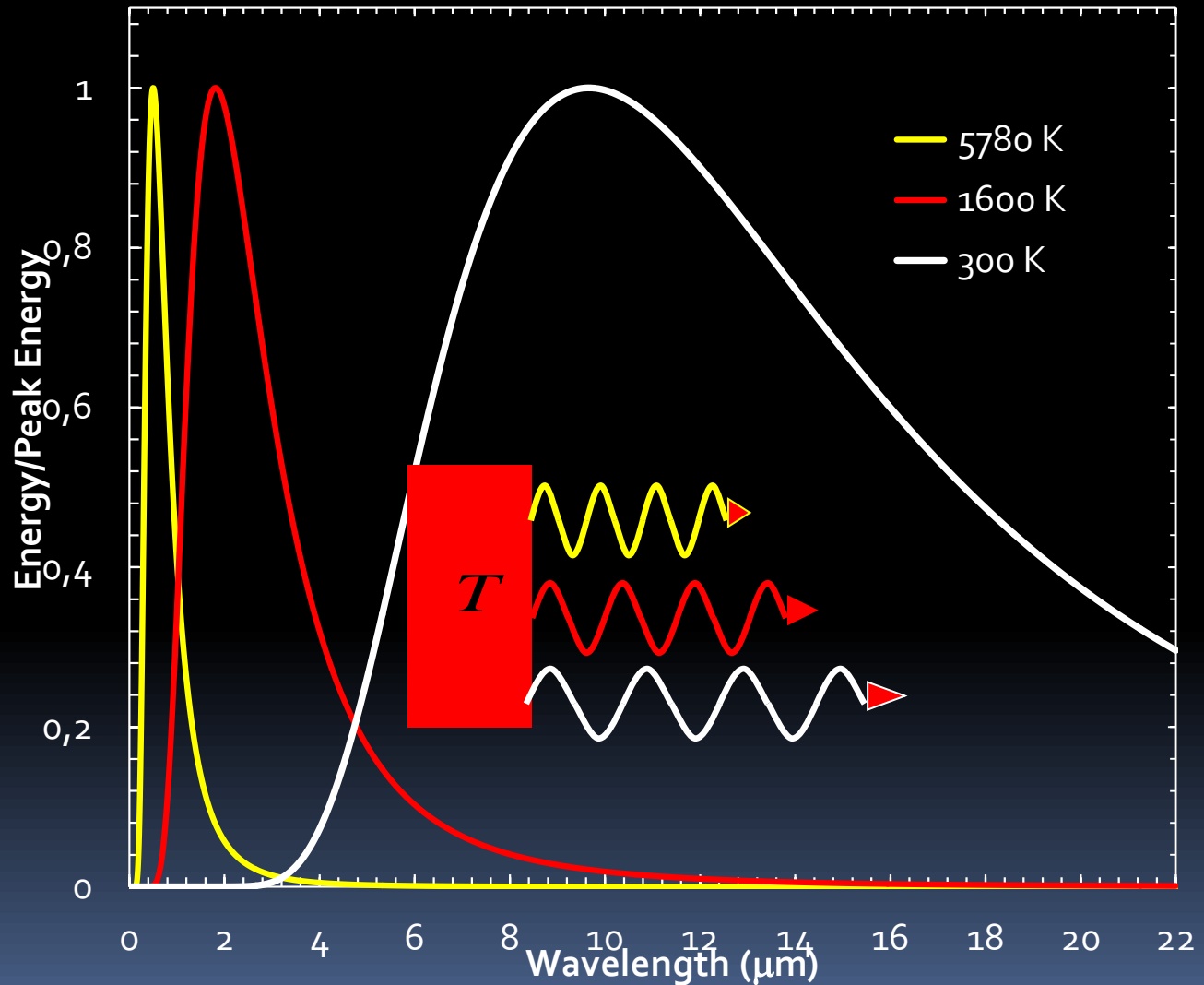
# Near Field Radiation Transfer @ Ozyegin Univ, Istanbul



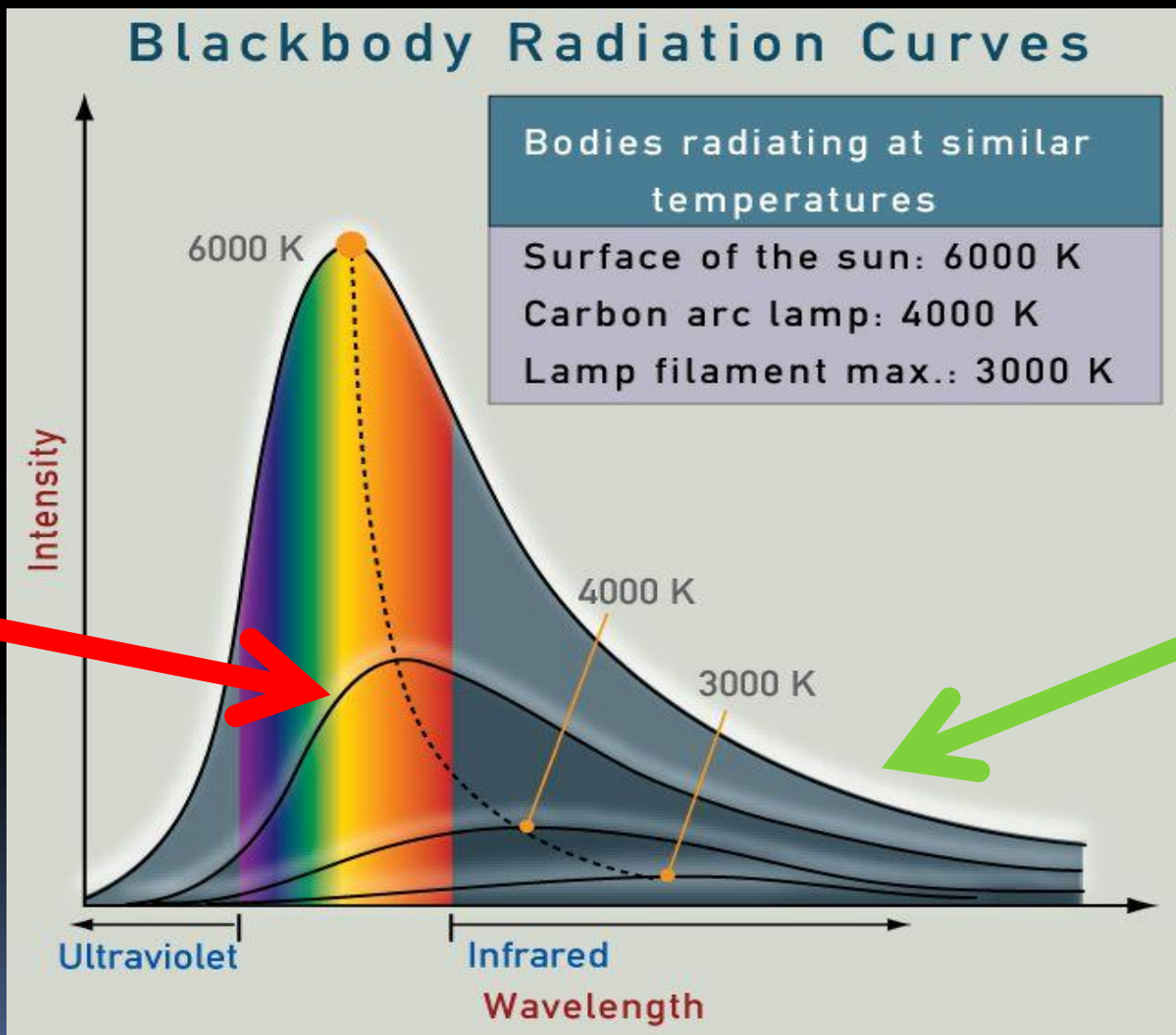
# PLANCK'S BLACKBODY RADIATION: BROADBAND



"Throughout the following discussion it will be assumed that the linear dimensions of all parts of space considered, [...], are large compared with the wavelengths of the rays considered."

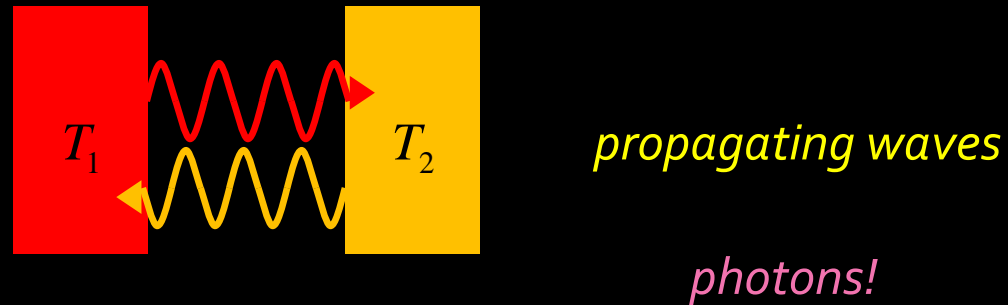


# RADIATIVE TRANSFER



# RADIATIVE TRANSFER

**RADIATION TRANSFER:** via electromagnetic waves



Maxwell's Equations fully describe the propagation of electromagnetic waves in all types of media.

Since the late 1800's, emission of radiation and radiation transfer were sufficiently explained by **Kirchhoff's** and **Planck's** Laws at the far-field.

Far-field radiation transfer is all about the microscopic space-time fluctuation of charge carriers. **Temperature** of the emitting body determines the spectral nature of thermal radiation.

# RADIATIVE TRANSFER

Energy transfer by electromagnetic waves!

Follows Planck's Blackbody Law

Long range ... No medium is required

**Scalable**.... if the distance between objects more than wavelength of radiation

- What happens if the objects are closer than the wavelength?
- What if the objects have structures on them?
- What if there are new materials to be used?
- Can we model and measure them?
- Can we come out with a device?

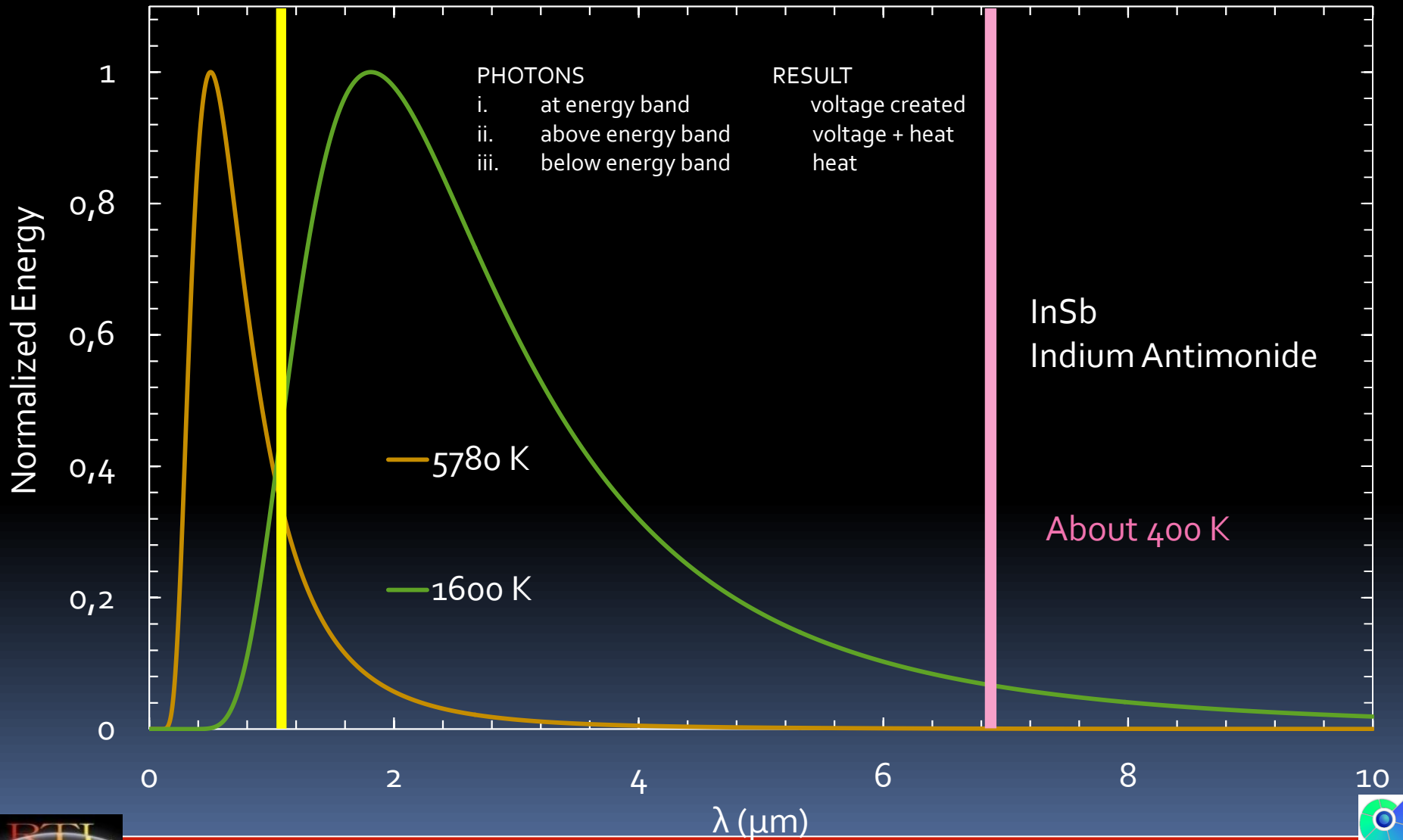
➤ **NANO-GAP THERMOHOTOVOLTAIC (n-TPV) CELL**

# RADIATIVE TRANSFER

About 3000 K

Si Band Gap: 1.12 eV or 1.1  $\mu\text{m}$

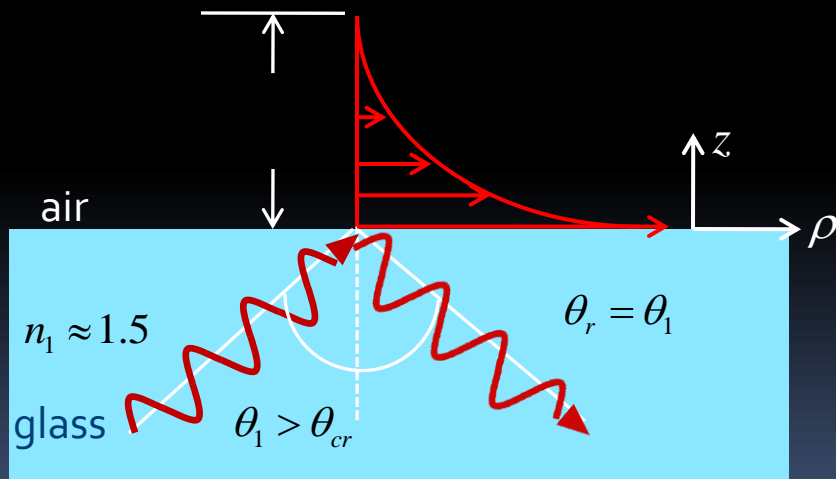
InSb Band Gap: 0.17 eV or 7.29  $\mu\text{m}$



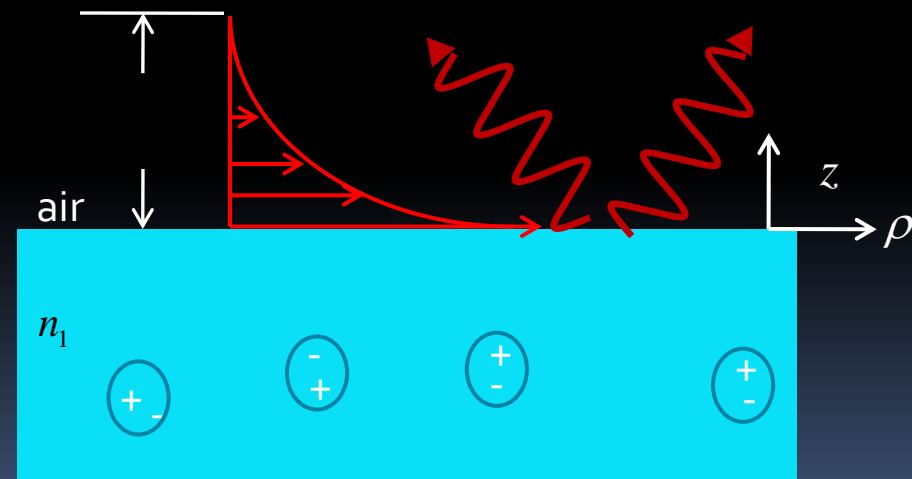
# EVANESCENT WAVES: FRUSTRATED TIR

Evanescent waves on the surfaces (e.g., due to total internal reflection).

Thermal near-fields and near-field spectral energy density are associated with the **intrinsic** electronic and vibrational excitations or **extrinsic** geometric resonances.



*total internal reflection (TIR)*



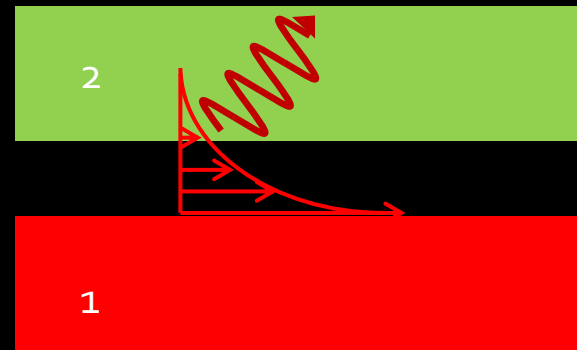
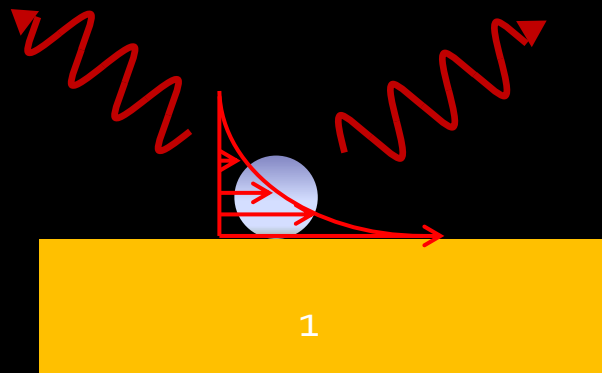
*dipole oscillations*

[Jackson, 1999; Hecht, 2002]



# NEAR-FIELD REGIME OF THERMAL RADIATION

What happens if a structure **interacts** with an evanescent wave?



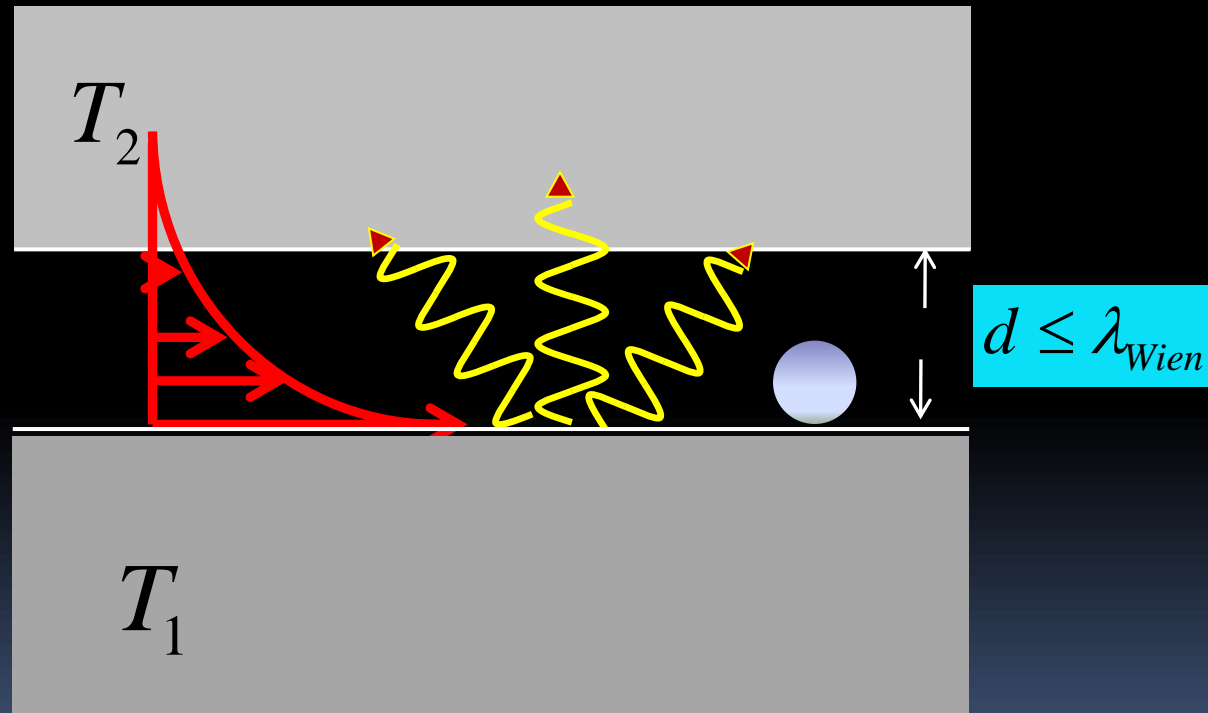
Two regimes of radiative transfer:

- **Far-field regime:** energy transfer via only propagating electromagnetic waves
- **Near-field regime:** energy transfer via both **evanescent** and propagating EM waves

(Francoeur, Mengüç)

# NEAR-FIELD RADIATION

How to calculate and measure radiative energy transfer between two objects in close proximity to each other?

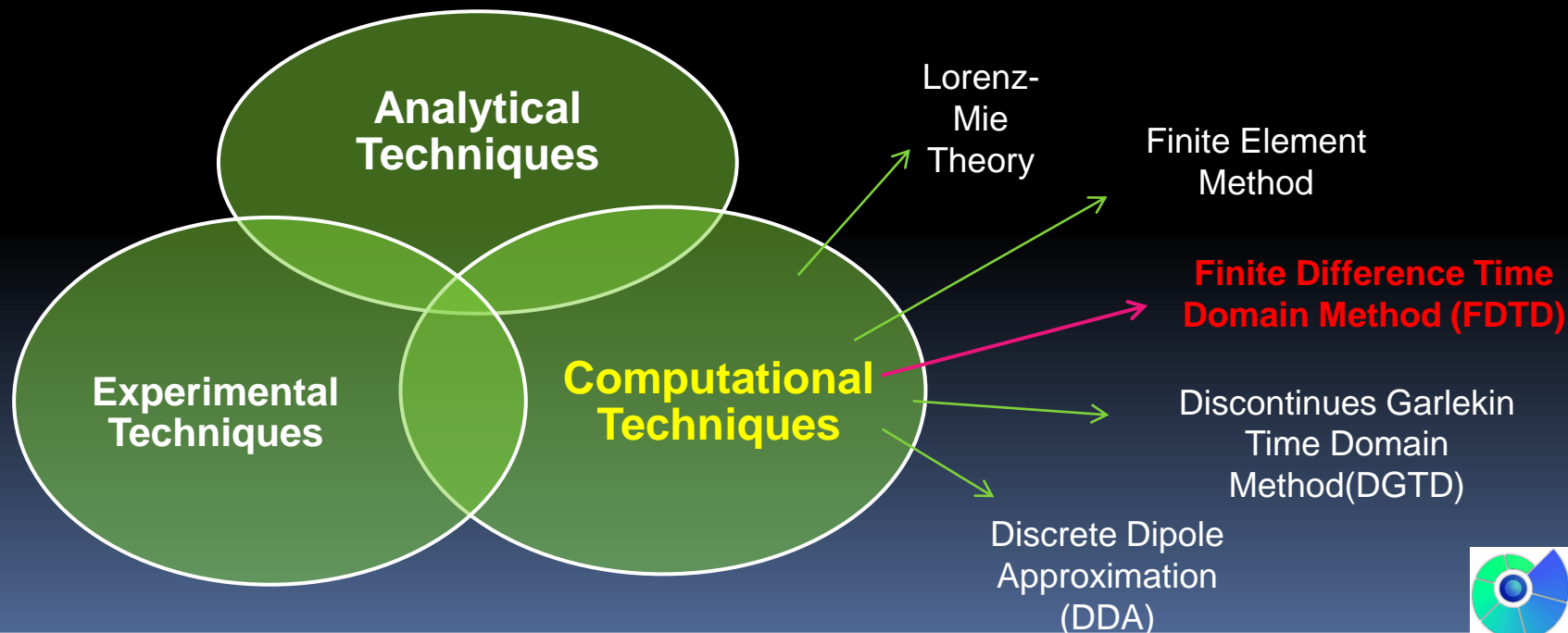


(Francoeur, Mengüç)

# Near field TPVs (Nano TPVs)

**Near field TPVs (Nano TPVs)** : By approaching a photovoltaic (PV) cell in proximity of a thermal emitter, thermal energy can be extracted by photon tunneling toward the cell...these devices are called Near-filed thermophotovoltaics (**NTPVS**).

## Modeling NTPVS :



# NEAR-FIELD RADIATION ANALYTICAL ANALYSIS

# NEAR-FIELD RADIATION TRANSFER

Maxwell's equations are valid to describe the propagation of electromagnetic waves at all scales (until the definitions of dielectric constant and magnetic permeability fails...down to a few nanometers).

However, thermal emission is not accounted for in the formulation of MEs.

Temperature of the medium can be entered to the MEs as a source term using **the fluctuation-dissipation theorem (FDT)**.

**FDT** incorporates the statistical properties of the current-density distribution.

# NEAR-FIELD REGIME OF THERMAL RADIATION

Maxwell equations combined with **fluctuational electrodynamics**

[Rytov, 1959; Francoeur and Mengüç, *JQSRT*, 2008; Francoeur et al., *JQSRT*, 2009]

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

$$\nabla \times \mathbf{H}(\mathbf{r}, \omega) = -i\omega \hat{\epsilon} \mathbf{E}(\mathbf{r}, \omega) + \mathbf{J}^r(\mathbf{r}, \omega)$$

$$\nabla \cdot \mathbf{D}(\mathbf{r}, \omega) = \nabla \cdot (\hat{\epsilon} \mathbf{E}(\mathbf{r}, \omega)) = \rho_e$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, \omega) = \nabla \cdot (\mu_0 \mathbf{H}(\mathbf{r}, \omega)) = 0$$

source of thermal radiation  
(stochastic current density)

Temperature of the medium correlated with  $\mathbf{J}^r$  via **the fluctuation-dissipation theorem**  
isotropic media

$$\langle J_\alpha^r(\mathbf{r}', \omega) J_\beta^{r*}(\mathbf{r}'', \omega) \rangle = \frac{\omega \epsilon_v \epsilon_r''(\omega)}{\pi} \Theta(\omega, T) \delta_{\alpha\beta} \delta(\mathbf{r}' - \mathbf{r}'')$$

mean energy of a Planck  
oscillator in thermal equilibrium

locality of the dielectric constant

(Francoeur, Mengüç)

# NEAR-FIELD REGIME OF THERMAL RADIATION

- Radiative heat flux (time-average Poynting vector):

$$\langle \mathbf{S}(\mathbf{r}, \omega) \rangle = 2 \operatorname{Re} \int_V dV^c \int_V dV^b \left[ \hat{\mathbf{x}}(G_{ya}^E G_{zb}^{H*} - G_{za}^E G_{yb}^{H*}) \hat{\mathbf{y}}(G_{za}^E G_{xb}^{H*} - G_{xa}^E G_{zb}^{H*}) + \hat{\mathbf{z}}(G_{xa}^E G_{yb}^{H*} - G_{ya}^E G_{xb}^{H*}) \right] \langle J_a^r(\mathbf{r}^c, \omega) J_b^{r*}(\mathbf{r}^b, \omega) \rangle$$

- Fluctuation-dissipation theorem:

$$\langle J_a^r(\mathbf{r}^c, \omega) J_b^{r*}(\mathbf{r}^b, \omega) \rangle = \frac{\omega e_v}{\rho} \operatorname{Im} \{ e_r(\omega) \} Q(\omega, T) d_{ab} d(\mathbf{r}^c - \mathbf{r}^b)$$

isotropic media

absorption/dissipation of thermal radiation

locality of the dielectric function

- General expression for the radiative heat flux:

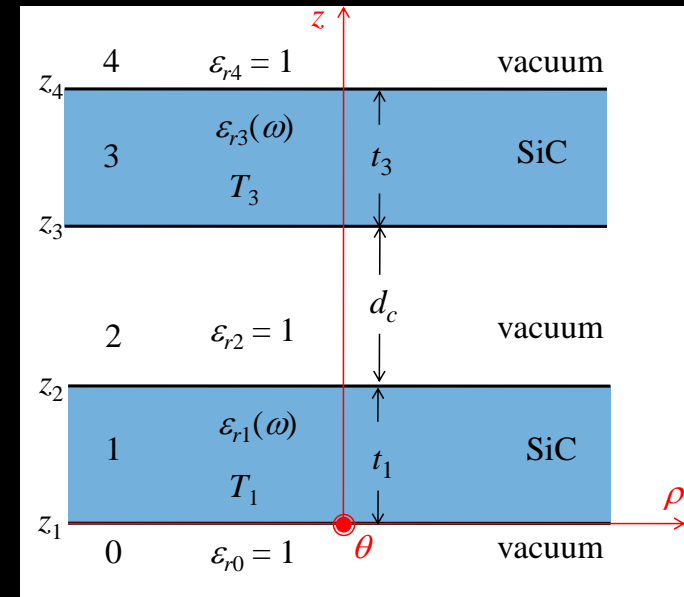
$$\langle \mathbf{S}(\mathbf{r}, \omega) \rangle = \frac{2k_v^2 Q(\omega, T)}{\rho} \operatorname{Re} \int_V dV^c \int_V dV^b \left[ \hat{\mathbf{x}}(G_{ya}^E G_{zb}^{H*} - G_{za}^E G_{yb}^{H*}) \hat{\mathbf{y}}(G_{za}^E G_{xb}^{H*} - G_{xa}^E G_{zb}^{H*}) + \hat{\mathbf{z}}(G_{xa}^E G_{yb}^{H*} - G_{ya}^E G_{xb}^{H*}) \right]$$

# NEAR-FIELD THERMAL RADIATION EMISSION

**Near-field radiative heat flux** between two thin films

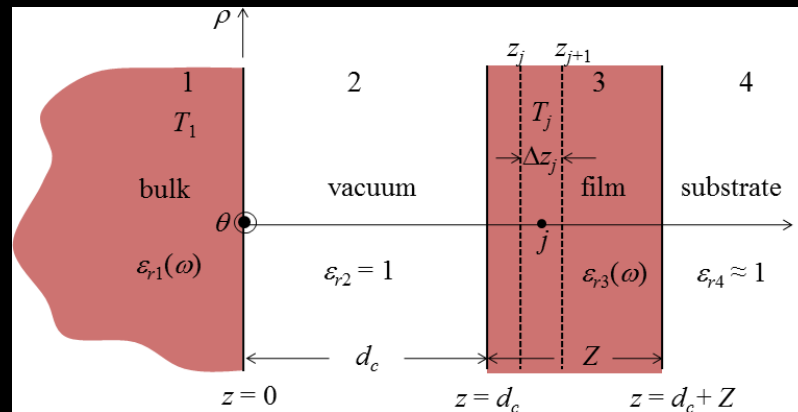
$$q_{\omega,abs} = q_{\omega,abs}^{prop} + q_{\omega,abs}^{evan}$$

$$q_{\omega,abs}^{evan} = \frac{\Theta(\omega, T_1)}{\pi^2} \int_{k_v}^{\infty} k_{\rho} dk_{\rho} e^{-2k_{z2} d_c} \sum_{\gamma=TE, TM} \frac{\text{Im}(R_1^{\gamma}) \text{Im}(R_3^{\gamma})}{|1 - R_1^{\gamma} R_3^{\gamma} e^{2ik_{z2} d_c}|^2}$$



$$q_{\omega,abs}^{prop} = \frac{\Theta(\omega, T_1)}{4\pi^2} \int_0^{k_v} k_{\rho} dk_{\rho} \sum_{\gamma=TE, TM} \frac{(1 - |R_1^{\gamma}|^2 - |T_1^{\gamma}|^2)(1 - |R_3^{\gamma}|^2 - |T_3^{\gamma}|^2)}{|1 - R_1^{\gamma} R_3^{\gamma} e^{2ik_{z2} d_c}|^2}$$

# NEAR-FIELD REGIME OF THERMAL RADIATION

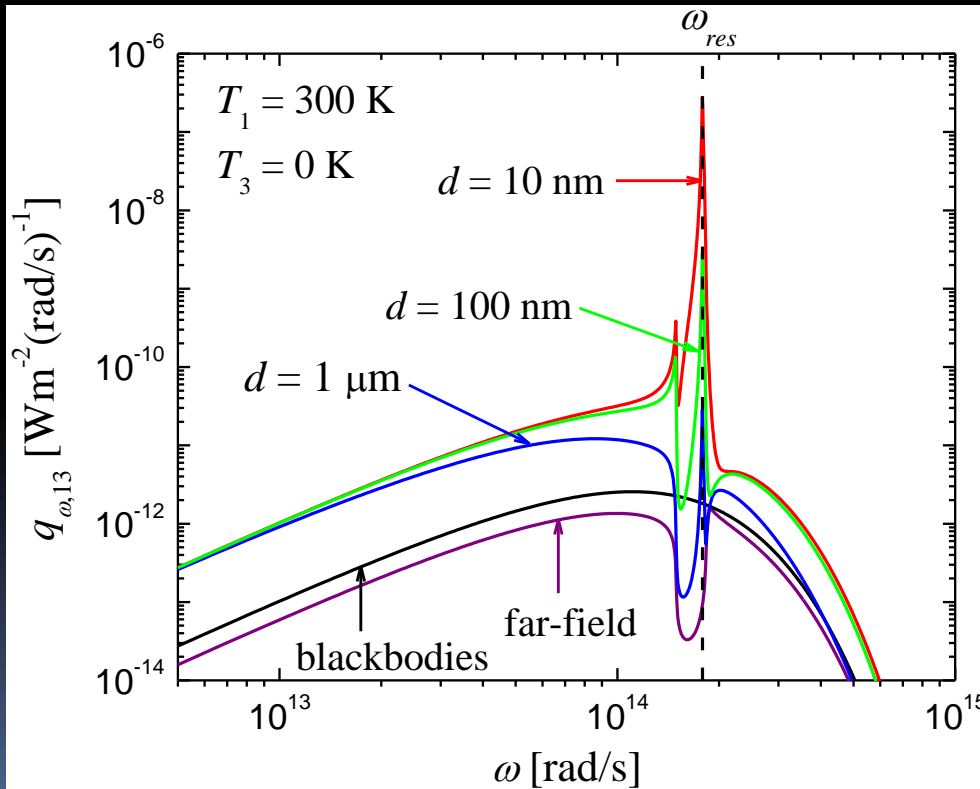
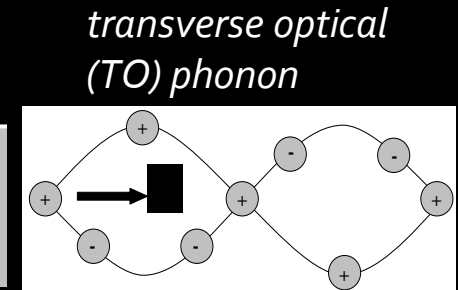
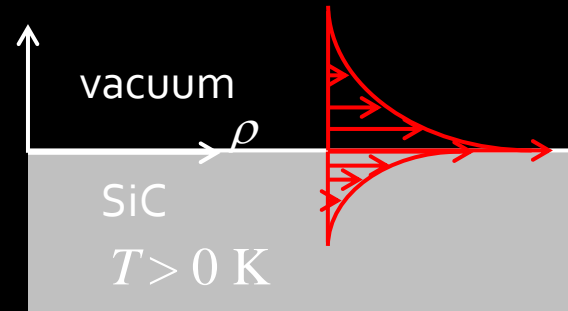
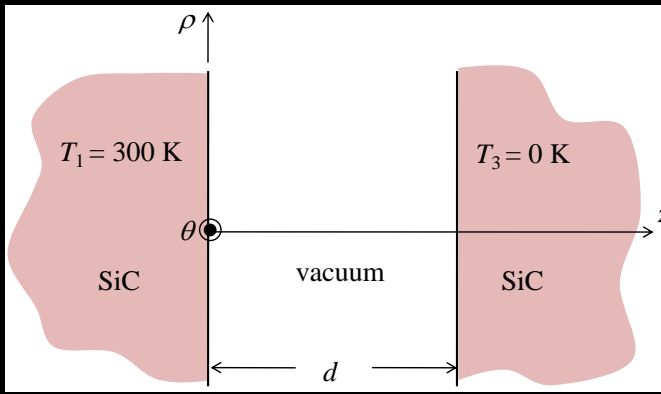


- Total net flux between medium 1 and control volume  $\Delta z_j$  in medium 3:

$$q_{\Delta z_j}^{abs} = \frac{W^2}{2\rho^2 c_v^2} \int_{W=0}^{\infty} dW [Q(W, T_1) - Q(W, T_j)]$$

$$\times \text{Re} \left\{ i e_{r_1}''(W) \int_{b=0}^{\infty} \frac{b db}{g_1''} \left[ \begin{array}{l} \left( \begin{array}{l} g_{13ra}^E(b, z_j, W) g_{13qa}^{H*}(b, z_j, W) \\ - g_{13qa}^E(b, z_j, W) g_{13ra}^{H*}(b, z_j, W) \end{array} \right) \\ - \left( \begin{array}{l} g_{13ra}^E(b, z_{j+1}, W) g_{13qa}^{H*}(b, z_{j+1}, W) \\ - g_{13qa}^E(b, z_{j+1}, W) g_{13ra}^{H*}(b, z_{j+1}, W) \end{array} \right) \end{array} \right] \right\}$$

# NEAR-FIELD THERMAL RADIATION BETWEEN TWO-FILMS



surface phonon-polaritons (SPhPs)  
supported by polar crystals (SiC, cBN,...)

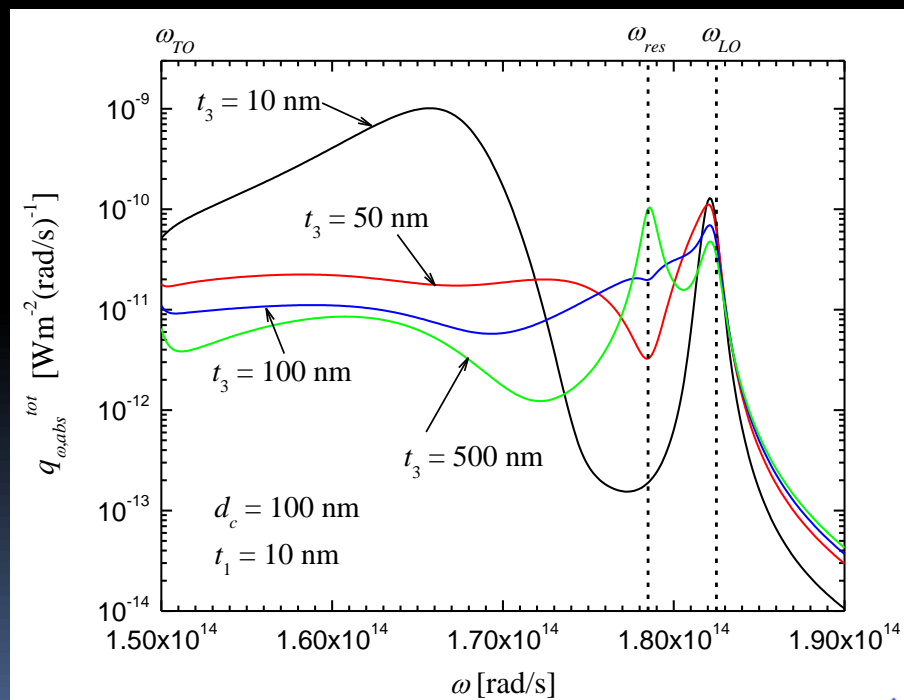
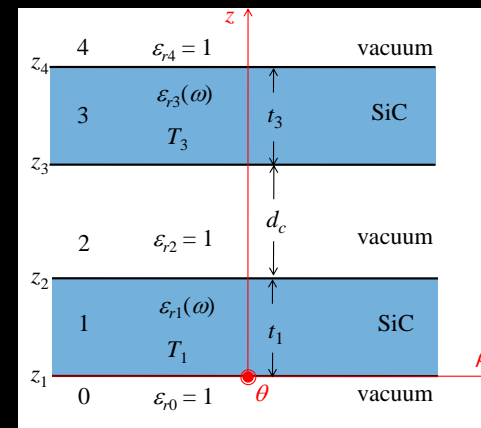
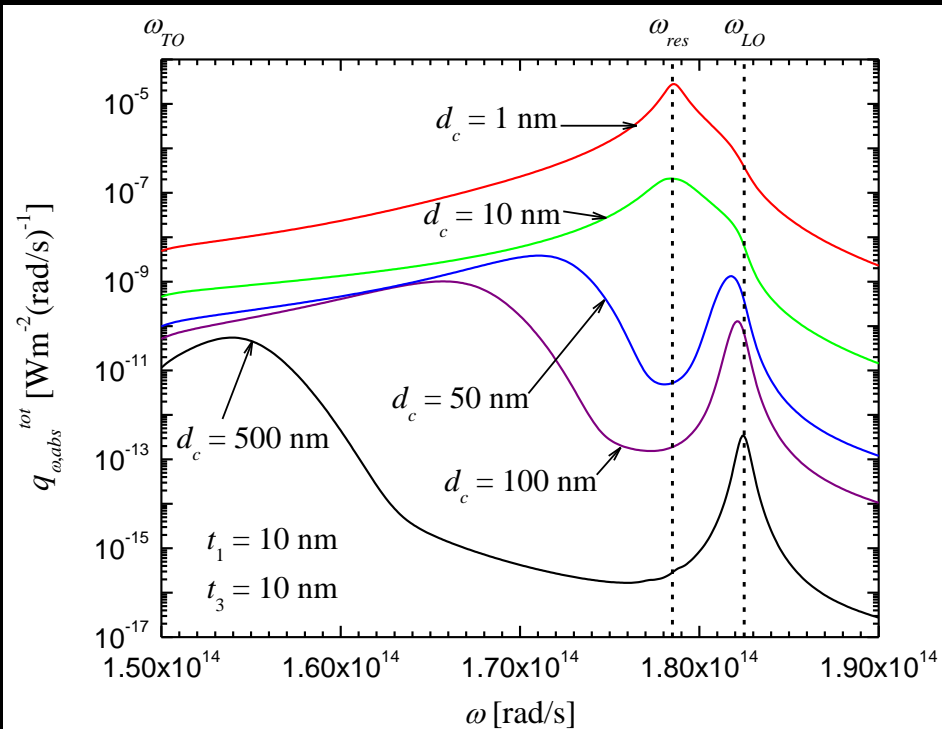
$$\omega_{res} = 1.786 \times 10^{14} \text{ rad/s}$$

$$= 10.55 \mu\text{m}$$

about 96-97% of the flux  
concentrated around  $\omega_{res}$

[Mengüç and Francoeur, *Thermal Radiation Heat Transfer*, Chapter 16, 2010]

# NEAR-FIELD THERMAL RADIATION BETWEEN TWO-FILMS



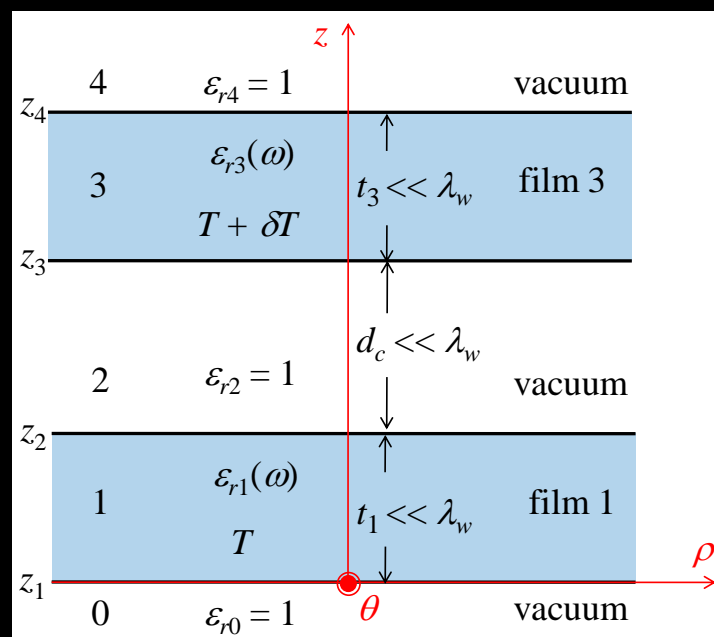
Francoeur, Mengüç, Vaillon, *J. Phys. D: Appl. Phys.*, 2010.

# COEXISTENCE OF MULTIPLE NEAR-FIELD RADIATION REGIMES

## RADIATIVE HEAT TRANSFER COEFFICIENT:

$k_r$  is the wavevector parallel to the surfaces of the layers,  $k_{z_j}$  is the z-component of the wavevector in medium  $j$ , and  $k_v$  is the magnitude of the wavevector in vacuum.

$T$  and  $R$  are the transmission and reflection coefficients of layer  $j$ , respectively, in polarization state  $\gamma$ .



$$h_r = \frac{1}{\pi^2} \int_0^\infty d\omega \frac{\partial \Theta(\omega, T)}{\partial T}$$

$$\times \sum_{\gamma=TE, TM} \left[ \int_0^{k_v} k_\rho dk_\rho \frac{(1 - |R_1^\gamma|^2 - |T_1^\gamma|^2)(1 - |R_3^\gamma|^2 - |T_3^\gamma|^2)}{4|1 - R_1^\gamma R_3^\gamma e^{2ik_{z2}d_c}|^2} + \int_{k_v}^\infty k_\rho dk_\rho e^{-2\text{Im}(k_{z2})d_c} \frac{\text{Im}(R_1^\gamma) \text{Im}(R_3^\gamma)}{|1 - R_1^\gamma R_3^\gamma e^{2ik_{z2}d_c}|^2} \right]$$

Francoeur, Mengüç, Vaillon, *Physical Review B*, Vol. 84, Issue: 7, Aug. 2011.

# COEXISTENCE OF MULTIPLE NEAR-FIELD RADIATION REGIMES

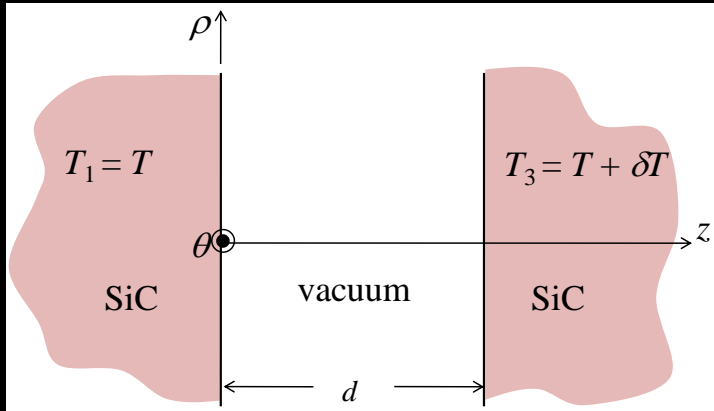
Approximate the Radiative Heat Transfer Coefficient

$$h_r \approx \frac{1}{\pi^2 d_c^2} \int_0^\infty d\omega \frac{\partial \Theta(\omega, T)}{\partial T} \int_0^\infty \eta e^{-2\eta} d\eta \frac{\text{Im}(R_1^{TM}) \text{Im}(R_3^{TM})}{|1 - R_1^{TM} R_3^{TM} e^{-2\eta}|^2}$$

Then, consider the asymptotic cases: e.g., For  $D$  much smaller than 1 ( $t \ll d$ )

$$h_r \approx \frac{1}{\pi^2 d_c^2} \int_0^\infty d\omega \frac{\partial \Theta(\omega, T)}{\partial T} \int_0^\infty \eta e^{-2\eta} d\eta \text{Im} \left( \frac{r_{01}^{TM}}{1 - (r_{01}^{TM})^2 (1 - 2\eta D_1)} \right) \text{Im} \left( \frac{r_{01}^{TM}}{1 - (r_{01}^{TM})^2 (1 - 2\eta D_3)} \right) \\ \times 4\eta^2 D_1 D_3 \frac{1}{\left| 1 - \frac{4\eta^2 D_1 D_3 (r_{01}^{TM})^2 e^{-2\eta}}{[1 - (r_{01}^{TM})^2 (1 - 2\eta D_1)][1 - (r_{01}^{TM})^2 (1 - 2\eta D_3)]} \right|^2}$$

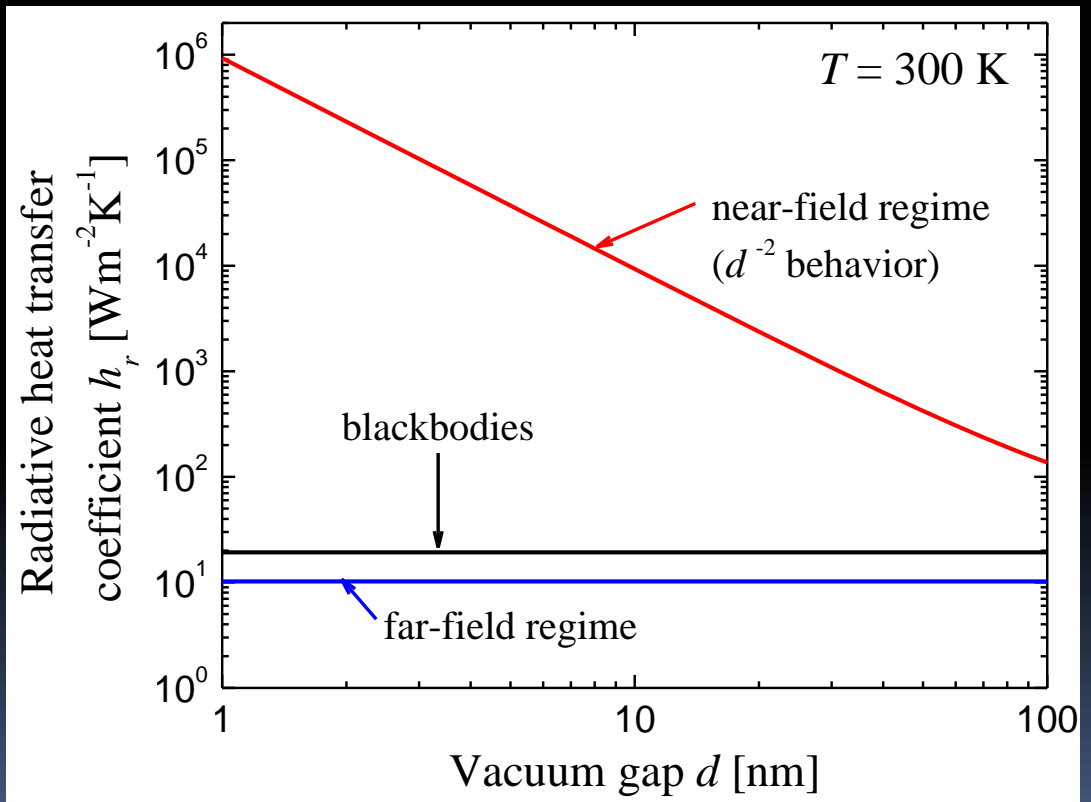
# NEAR-FIELD THERMAL RADIATION EMISSION FROM A SINGLE FILM



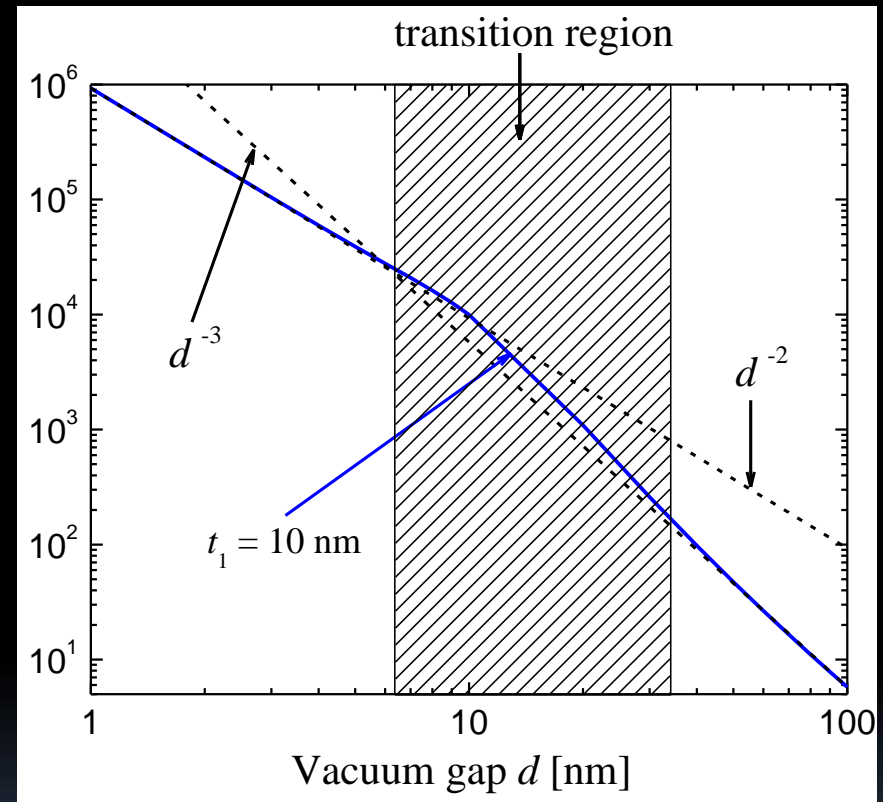
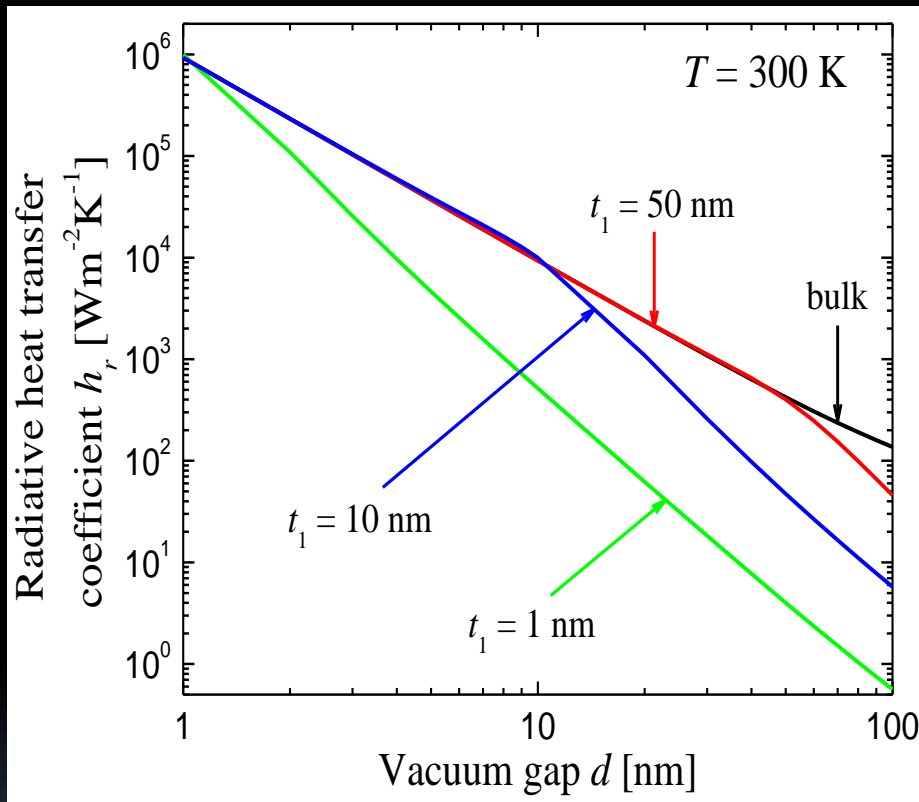
$$h_r = \lim_{\delta T \rightarrow 0} \frac{\int_0^{\infty} q_{\omega,13} d\omega}{\delta T}$$

$d = 10 \text{ nm}$ :

✓ Near-field radiative transfer coefficient  $\sim 500$  times blackbodies



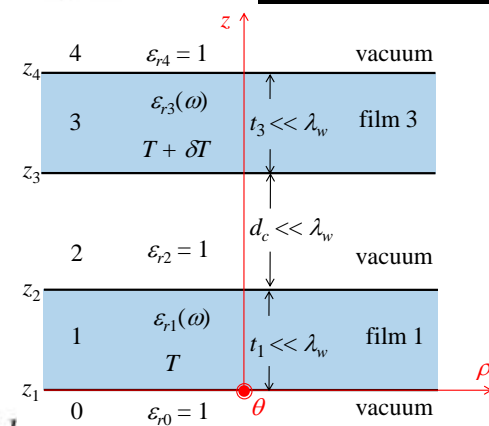
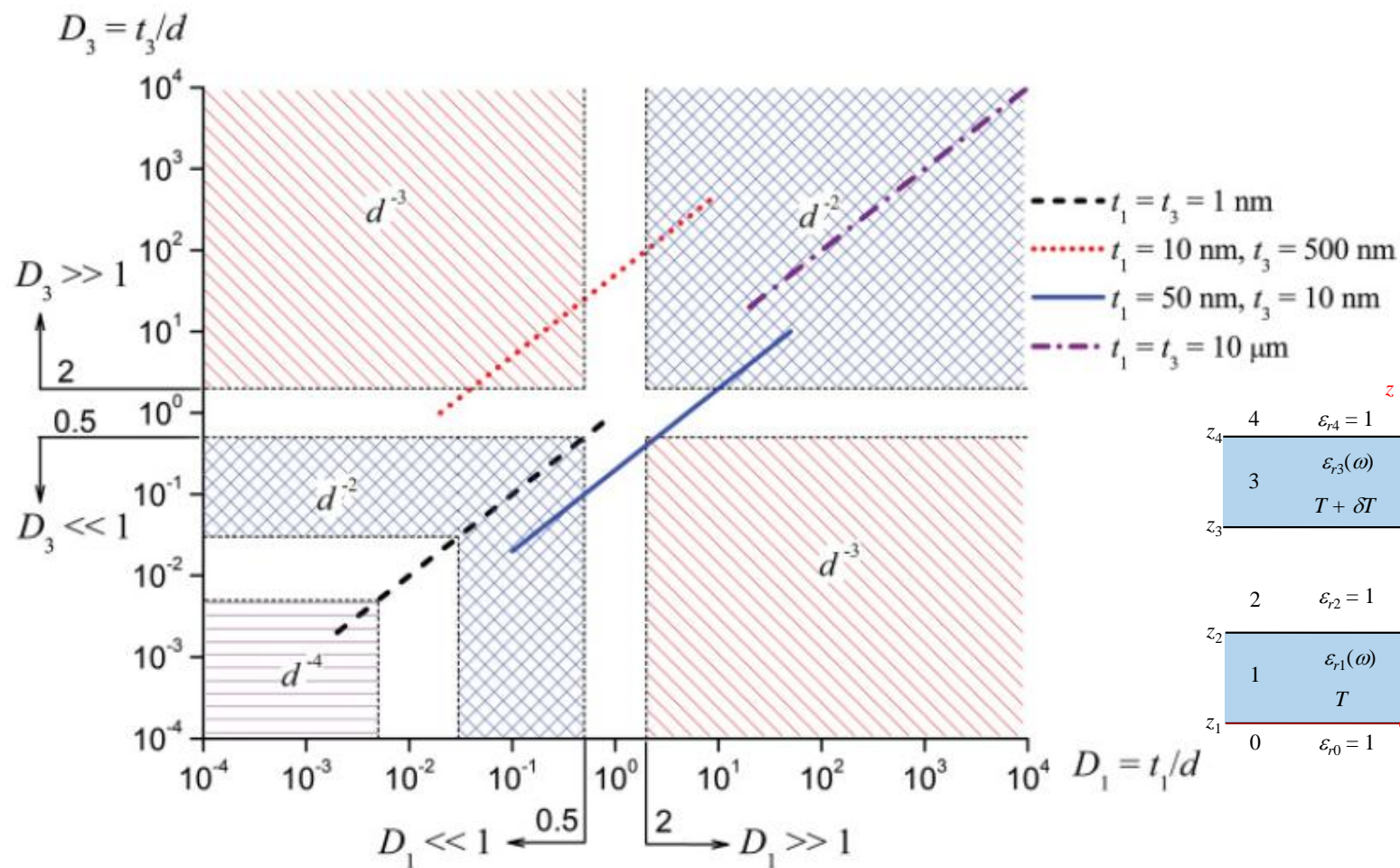
# COEXISTENCE OF MULTIPLE NEAR-FIELD RADIATION REGIMES



Coexistence of **two near-field thermal radiation regimes** due to surface phonon-polariton coupling within the emitter

Francoeur, Mengüç, Vaillon, *Physical Review B*, Vol. 84, Issue: 7, Aug. 2011.

# COEXISTENCE OF MULTIPLE NEAR-FIELD RADIATION REGIMES

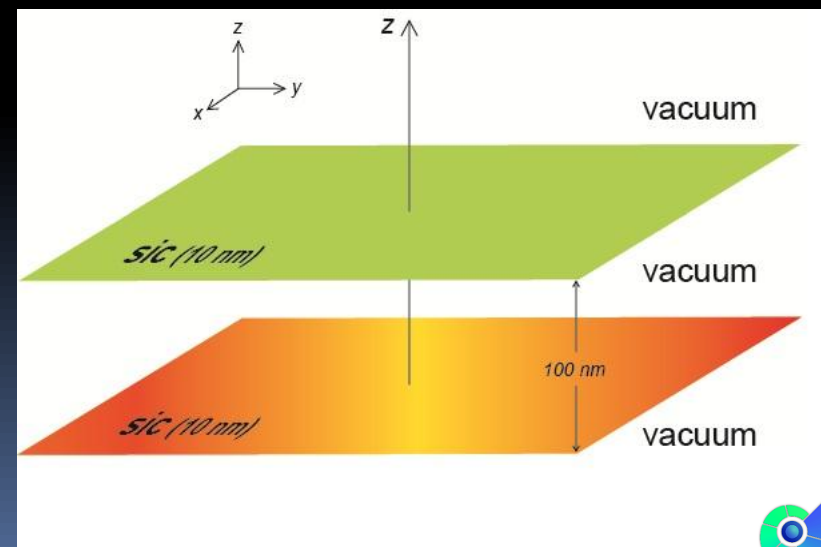


Francoeur, Mengüç, Vaillon, *Physical Review B*, Vol. 84, Issue: 7, Aug. 2011.

# NEAR-FIELD RADIATION COMPUTATIONAL ANALYSIS

- **FDTD (Finite Difference Time Domain Method)** is a computational method used to analyse electromagnetic wave propagation problems. It gives solution to **Maxwell's equations**. It is based on a computational grid.
- Two **Silicon Carbide films**, both supporting SPhP, each 10 nm thick, the lower film has ( $T > 0$  K) while the upper one ( $T = 0$  K). They are separated by vacuum gap of 100 nm thickness.
- **Local Density of Electromagnetic States (LDOS)** is calculated. This allows us to calculate thermal radiation emission in the gap between the SiC layers.

Azadeh Didari, Mengüç, Ozyegin Univ, 2012



**Finite Difference Time Domain Technique** is a time domain technique which has been chosen as our computational method of choice:

**FDTD** is a time domain based numerical method, hence it has the capability to give us the solution of a **very wide band frequency range** within a **single run**.

**FDTD** can model various arbitrary geometries having different shapes and sizes whose analytical studies may not be available due to complexity of the problem is possible

**FDTD** can incorporate the effects of reflection and radiation which are commonly neglected by other methods

**FDTD** can model wave propagation in complex media, such as time-varying, anisotropic, lossy, dispersive and non-linear media is possible.

## The 1D-FDTD Equations

We start by Maxwell equations:

$\mathbf{D}$ ,  $\mathbf{H}$ , and  $\mathbf{E}$  are vectors in three dimensions. We will start with 1D case using  $D_x$  and  $H_y$  and denoting the plane wave in  $z$  direction.

In order to apply the PML ABC we use the following equations:

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H}$$

$$\mathbf{D}(\omega) = \varepsilon_0 \varepsilon_r(\omega) \mathbf{E}(\omega)$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E}$$

$$\frac{\partial D_x}{\partial t} = -\frac{\partial H_y}{\partial z}$$

$$D_x(\omega) = \varepsilon_0 \varepsilon_r(\omega) E_x(\omega)$$

$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_x}{\partial z}$$

$$\frac{\partial D_x}{\partial t} + \frac{\sigma D_x}{\varepsilon_0} = -\frac{\partial H_y}{\partial z}$$

$$D_x(\omega) = \varepsilon_0 \varepsilon_r(\omega) E_x(\omega)$$

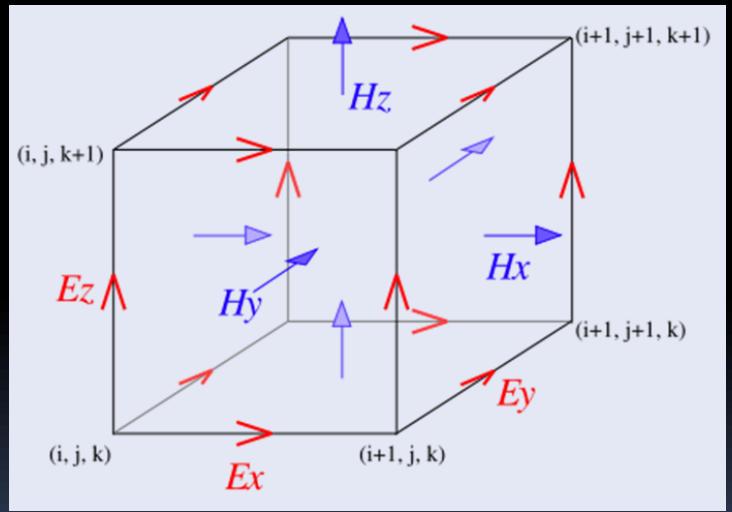
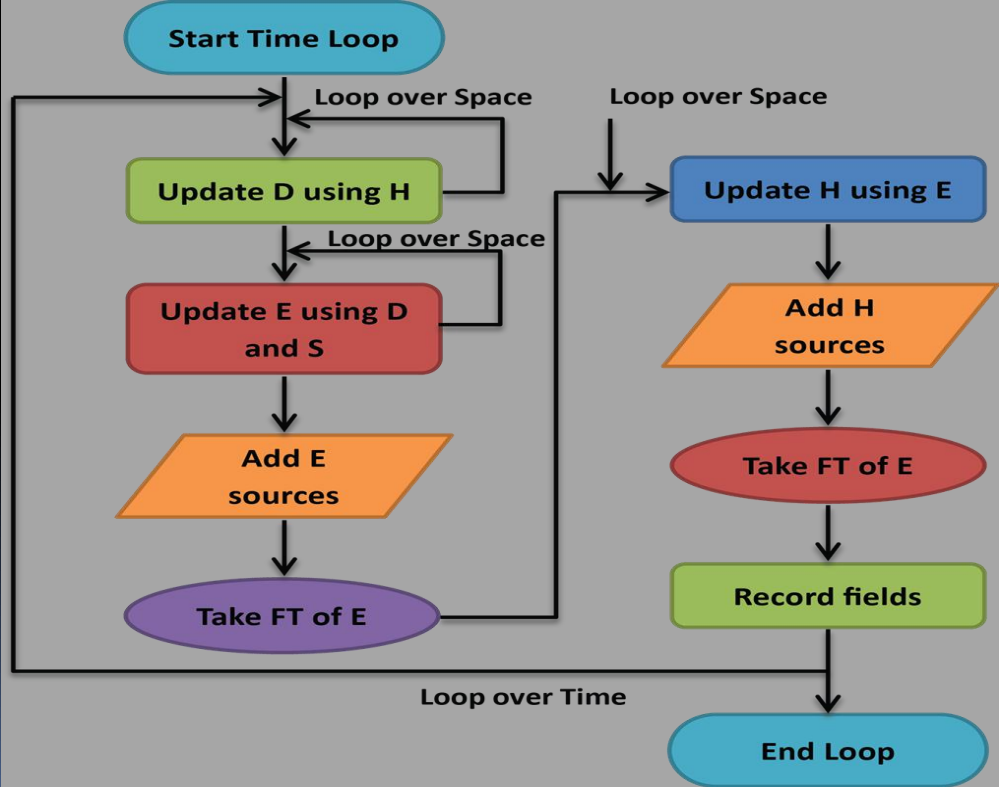
$$\frac{\partial H_y}{\partial t} + \frac{\sigma^* H_y}{\mu_0} = -\frac{1}{\mu_0} \frac{\partial E_x}{\partial z}$$

Where  $\sigma$  and  $\sigma^*$  are respectively the electric conductivity and the magnetic conductivity of the PML medium with  $\sigma/\varepsilon_0 = \sigma^*/\mu_0$ . In order to produce a smooth transition from air cells to the PML cells, the conductivity is gradually increased from zero at the vacuum-layer interface to a maximum value of  $\sigma^*$  for each layer.  $\sigma(\rho) = \sigma_m (\rho/\delta)^2$

# Computational Techniques : Finite Difference Time Domain Method (FDTD)

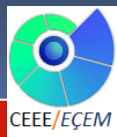
## How does FDTD work?

Using **Yee cells** as discrete units, **Maxwell's equations** are converted to a set of **central difference** equations which are to be solved in each Yee unit cell according to the following flowchart:



Yee Cell

Didari, Mengüç, 2013



## FDTD Requirements :

- **Boundary Conditions:**

Mur's first order ABC



Mei-Fang  
superabsorption



Conventional Perfectly  
Matched Layer(CPML)

Detailed **modeling** studies, and **accurate calculation** of near-field emission within thin films are necessary in order to calculate the **local density of electromagnetic states (LDOS)** which is a key factor to obtain the **radiation heat flux in near field thermal radiation** related problems.

## Numerical Dispersion:

Cell size

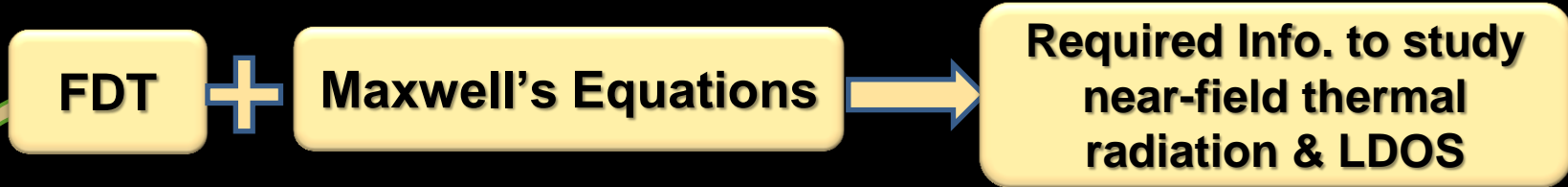


$\lambda_{\min} / 10$

Didari, Mengüç, 2013

# Modelling of Near-field thermal radiation within nano-gaps via FDTD... Fluctuation Dissipation Theorem (FDTD)...

The **fluctuation-dissipation theorem** is a general result of statistical thermodynamics that quantifies the relation between the fluctuations in a system at thermal equilibrium and the response of the system to applied perturbations



**FDT: Fluctuation  
dissipation theorem**

**TM evanescent component of monochromatic  
Local density of Electromagnetic state (LDOS)**

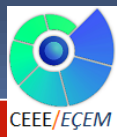
$$\rho_{\omega}(\mathbf{r}) = \frac{\omega \varepsilon_r''(\omega)}{\pi c_0^2} \left\{ k_v^2 \int_{V'} dV' \left( |G_{XX}^E|^2 + |G_{XZ}^E|^2 + |G_{ZX}^E|^2 + |G_{ZZ}^E|^2 \right) + \int_{V'} dV' \left( |G_{YX}^H|^2 + |G_{YZ}^H|^2 \right) \right\}$$

$$\langle J_{\alpha}^r(\mathbf{r}', \omega) J_{\beta}^{r*}(\mathbf{r}'', \omega') \rangle = \frac{\omega \varepsilon_0 \varepsilon_r''(\omega)}{\pi} \Theta(\omega, T) \delta(\mathbf{r}' - \mathbf{r}'') \delta(\omega - \omega') \delta_{\alpha\beta}$$

**Drude-Lorentz Model**

$$\varepsilon_r(\omega) = \varepsilon_{\infty} \frac{\omega^2 - \omega_{LO}^2 + i\Gamma\omega}{\omega^2 - \omega_{TO}^2 + i\Gamma\omega}$$

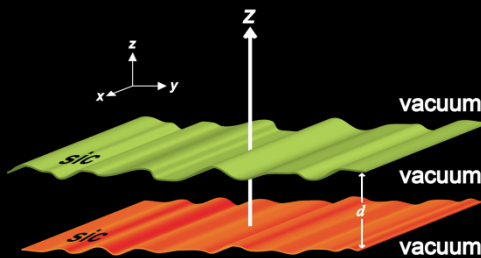
Didari, Mengüç, 2013



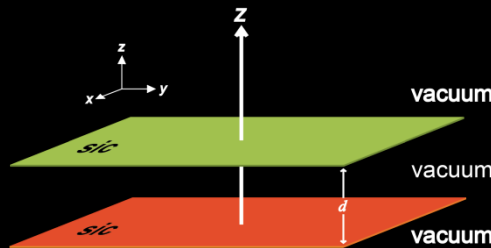
# Modelling of Near-field thermal radiation within nano-gaps via FDTD...

## ➤ Medium specifications :

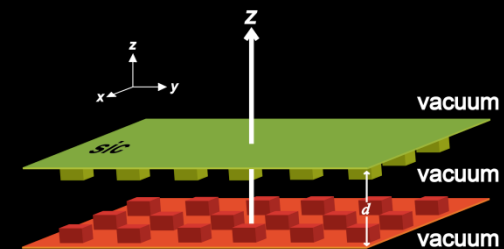
- Two Silicon Carbide films, both supporting SPhP, each 10 nm thick, the lower film has ( $T > 0$  K) while the upper one ( $T = 0$  K). They are initially separated by vacuum gap of 100 nm thickness.



**Realistic model**



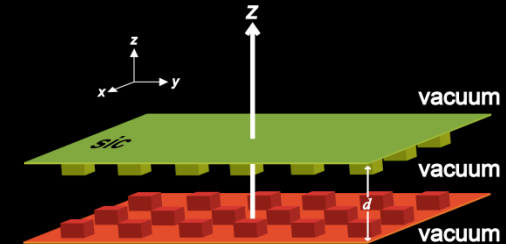
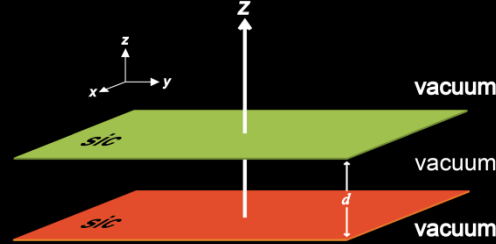
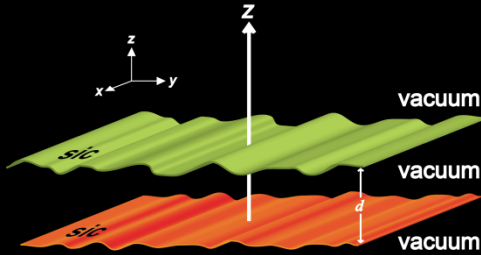
**Considered model**



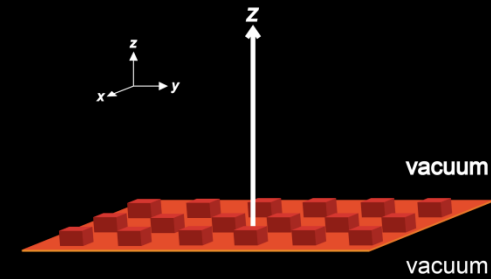
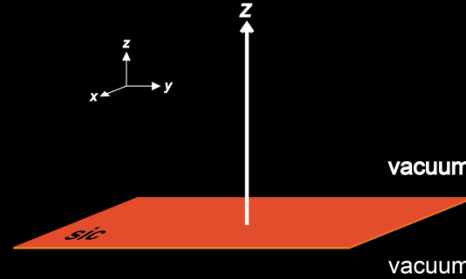
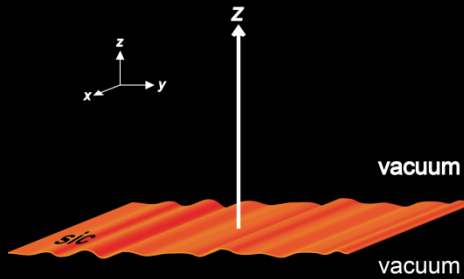
**Future model**

# Modelling of Near-field thermal radiation within via FDTD...

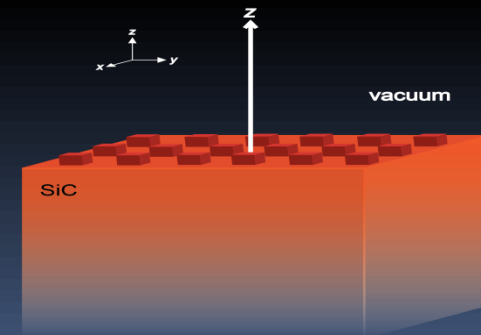
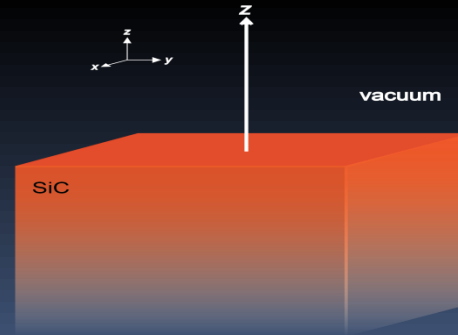
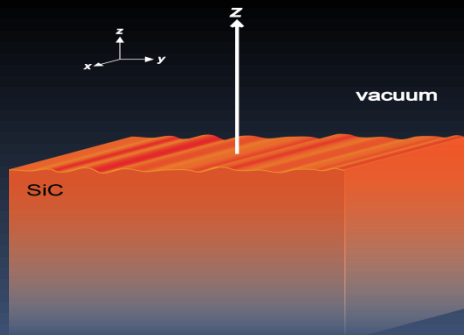
Thin films of metamaterial



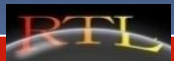
Single film of metamaterial



Bulk metamaterial

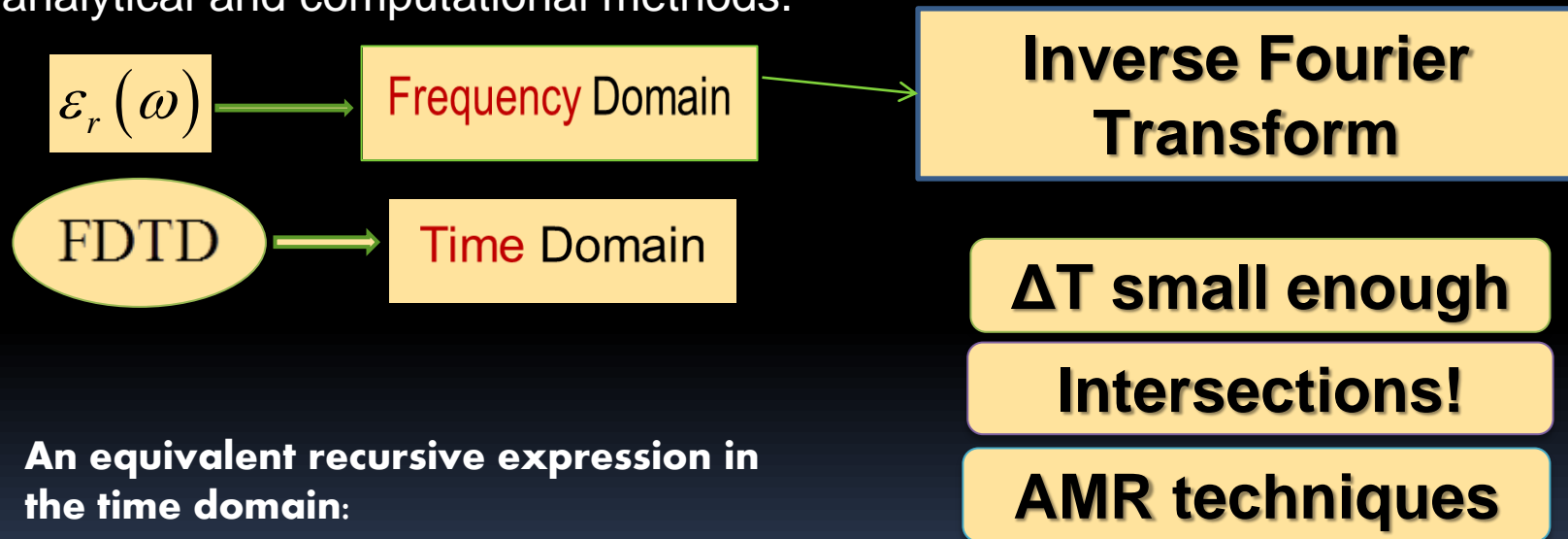


Didari, Mengüç, 2013



## Methodology

- A comparison has been made between Analytical results found previously by Francoeur et al., and the FDTD calculations developed. The results showed promising agreement between the analytical and computational methods.



**An equivalent recursive expression in the time domain:**

$$S^n = 2e^{-\alpha\Delta t} \cos(\beta\Delta t) S^{n-1} - e^{-2\alpha\Delta t} S^{n-2} + Ae^{-\alpha\Delta t} \sin(\beta\Delta t) E^{n-1}$$

$$\alpha = \Gamma / 2 \quad \beta = \sqrt{\omega_{TO}^2 - \Gamma^2 / 4} \quad A = \epsilon_0 \epsilon_\infty (\omega_{LO}^2 - \omega_{TO}^2) / \sqrt{\omega_{TO}^2 - \Gamma^2 / 4}$$

# Modelling of Near-field thermal radiation within nano-gaps via FDTD...

- LDOS is calculated in the **vacuum gap between two thin film** and compared to the analytical solution:

Thicknesses

Gap

Test Point

$$t_1 = 100 \text{ nm} , t_2 = 10 \text{ nm}$$

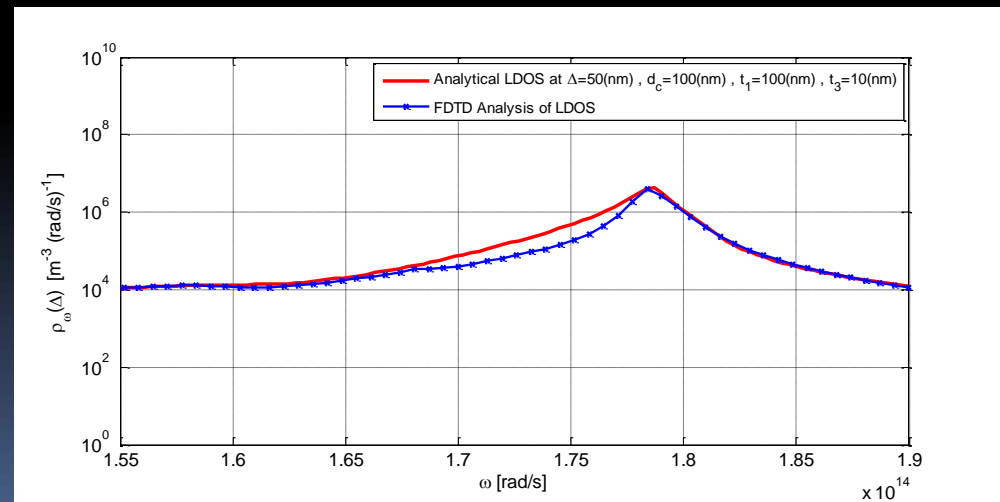
$$d = 100 \text{ nm}$$

$$\Delta = 50 \text{ nm}$$



Peak around :

$$\omega_{res} = 1.786 \times 10^{14} \text{ rad/s}$$



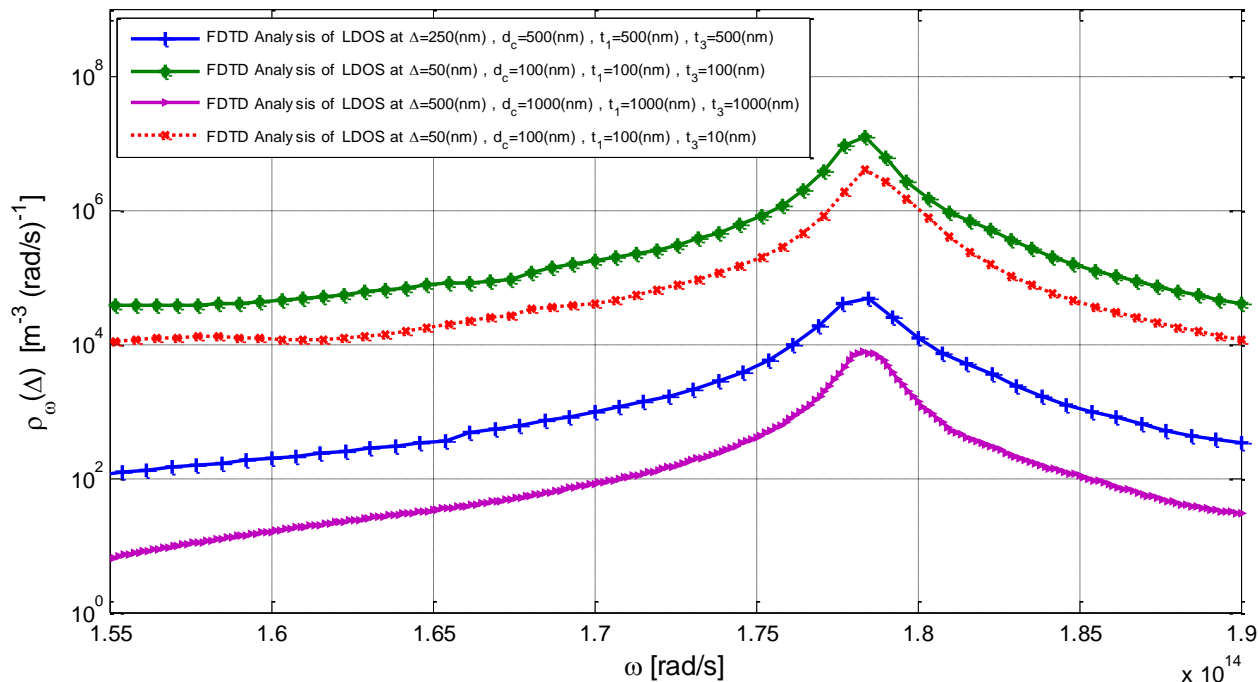
Didari, Mengüç, 2013

# Modelling of Near-field thermal radiation within nano-gaps via FDTD...

Didari, Mengüç, 2013

Study of the effect of the gap size on LDOS profile...

An increase of three orders of magnitude is observed when the gap size is below 500 nm



# What about arbitrary Geometries?

When it comes to arbitrary geometries e.g. A tip and a plate...

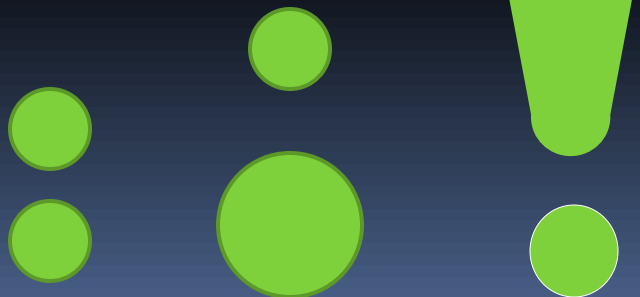
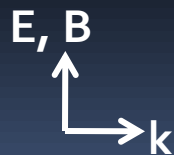
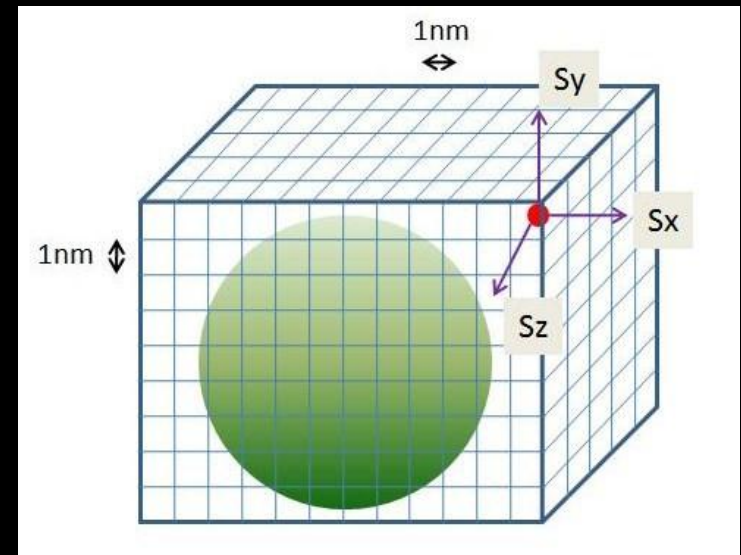
Use DDA-SI

Test FDTD for the same geometries and compare the results with DDA-SI results.

**RADIATION ABSORPTION AND SCATTERING  
BETWEEN CLOSE PARTICLES AND SURFACES**

# TWO PARTICLE INTERACTION

- Individual Absorptions
- Integrated Poynting Vector
  
- Geometries
  - Two Identical Spheres
  - Two Spheres with different sizes
  - Conical tip and a nanosphere



Donmezer, Okutucu, Mengüç

# DDA-SI: TO ACCOUNT FOR SURFACE EFFECTS RIGOROUSLY

- **D**iscrete **D**ipole **A**pproximation – **S**urface **I**nteraction
- Based on DDSURF, unreleased code by Schmehl et al.
- Prototype MATLAB implementation can be ported to C and Fortran if speed is required
- MATLAB has a very efficient numerical linear system solver (gmres)

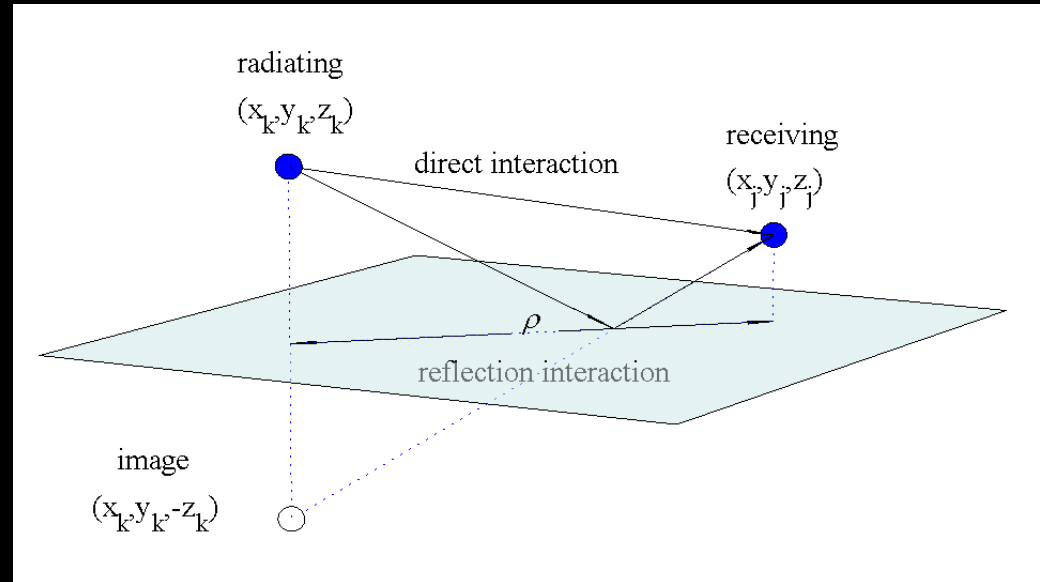
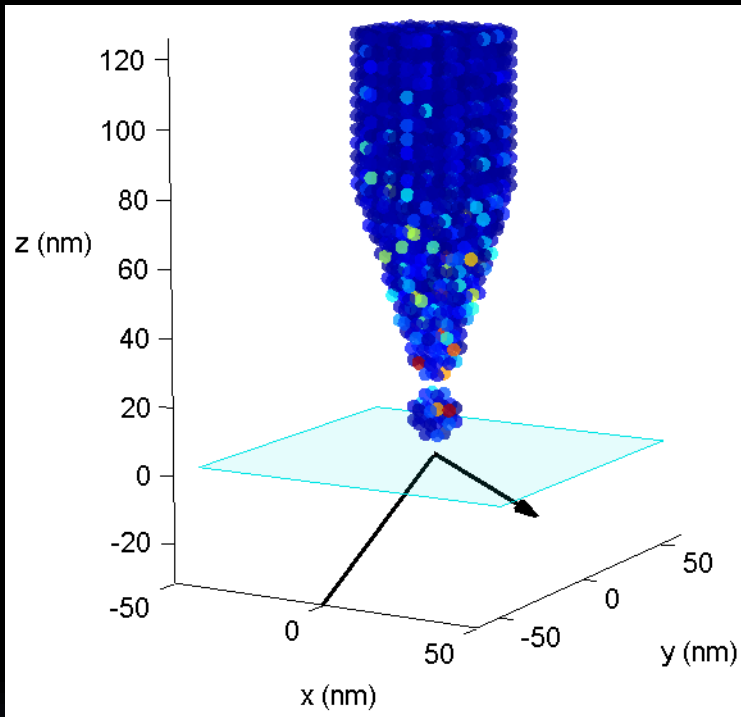
V. L. Y. Loke and M. P. Mengüç. "Surface waves and afm probe-particle near-field coupling: Discrete dipole approximation with surface interaction". *to appear in J. Opt. Soc. Am. A*, 2010.

R. Schmehl, B. M. Nebeker and E. D. Hirleman, "Discrete-dipole approximation for scattering by features on surfaces by means of a two-dimensional fast Fourier transform technique", *J. Opt. Soc. Am. A.* 14(11), 3026-3036 (1997).

Loke, Mengüç, 2010



# DDA-SI SYSTEM OF EQUATIONS



The interaction matrix now comprises the direct and reflected terms

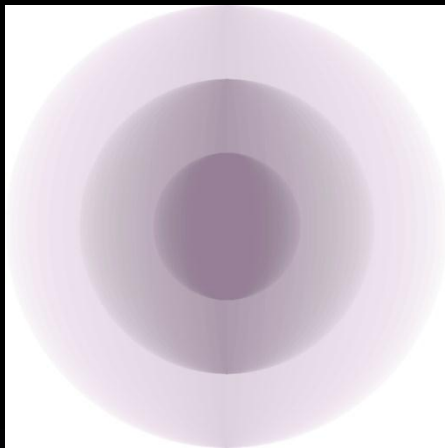
$$\sum_{k=1}^N \mathbf{A}_{jk}^{\text{SI}} \mathbf{P}_k = \mathbf{E}_{\text{inc},j}$$



$$\sum_{k=1}^N (\mathbf{A}_{jk} + \mathbf{R}_{jk}) \mathbf{P}_k = \mathbf{E}_{\text{inc},j}$$

# DECOMPOSING THE SPHERICAL WAVE

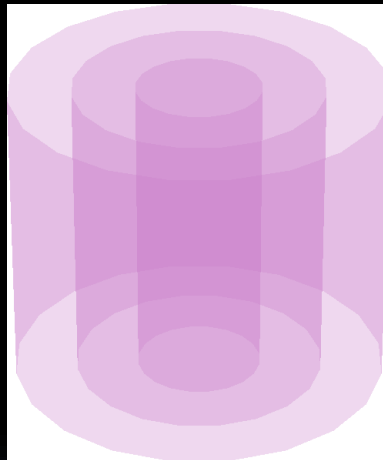
$$\left(\frac{e^{ikr}}{r}\right)_{ref} = i \int_0^\infty \frac{k_\rho}{k_z} J_0(k_\rho \rho) R_{21}^{TM,TE} e^{ik_z |z_j|} dk_\rho$$



$$\frac{e^{ikr}}{r}$$

Spherical

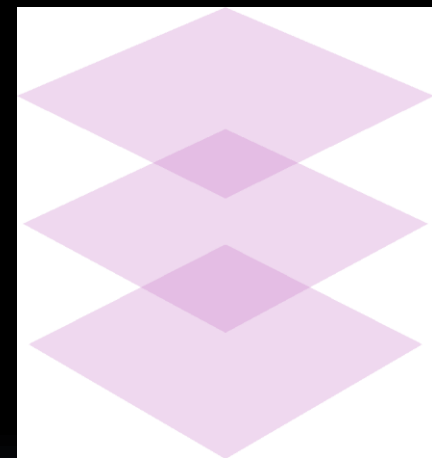
=



$$J_0(k_\rho \rho) \text{ or } \frac{1}{2} H_0^{(1)}(k_\rho \rho)$$

Cylindrical

+

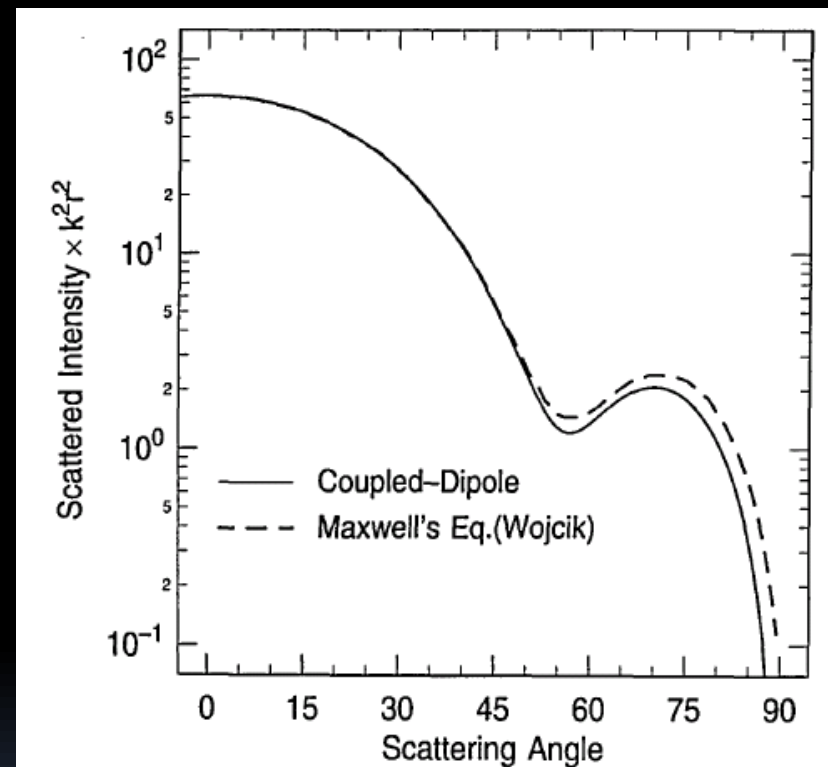
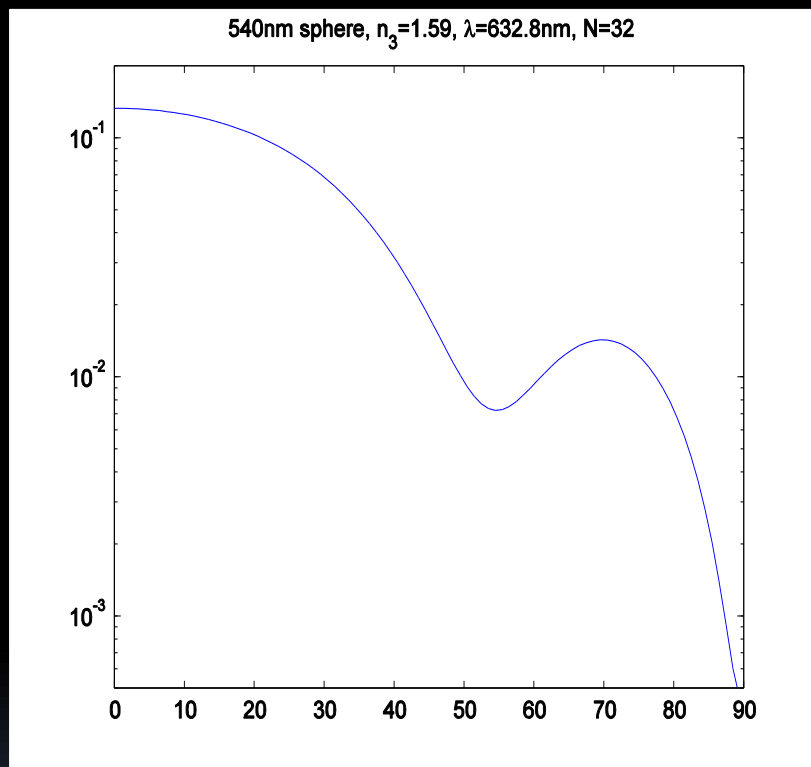


$$e^{ik_z |z|}$$

Planar

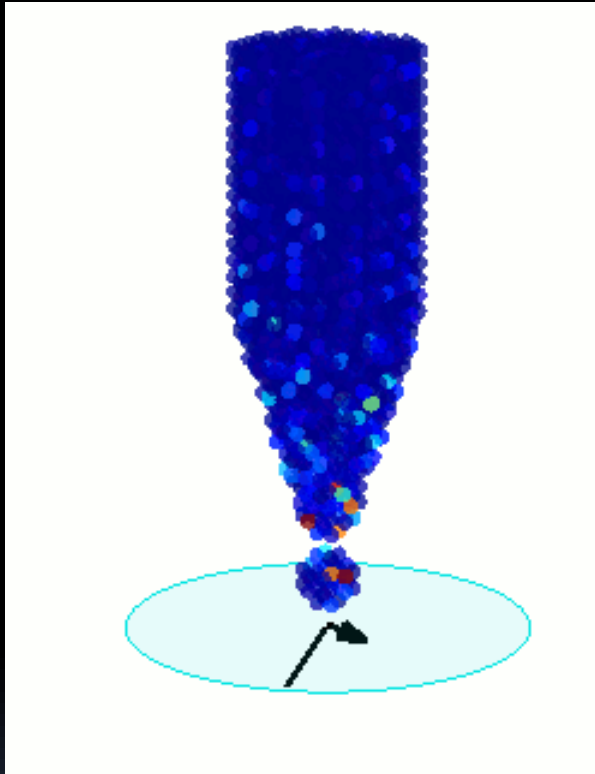
A. Sommerfeld, "Über die Ausbreitung der Wellen in der drahtlosen Telegraphie,"  
Ann. Physik 28, 665–737 (1909).

# Testing the implementation

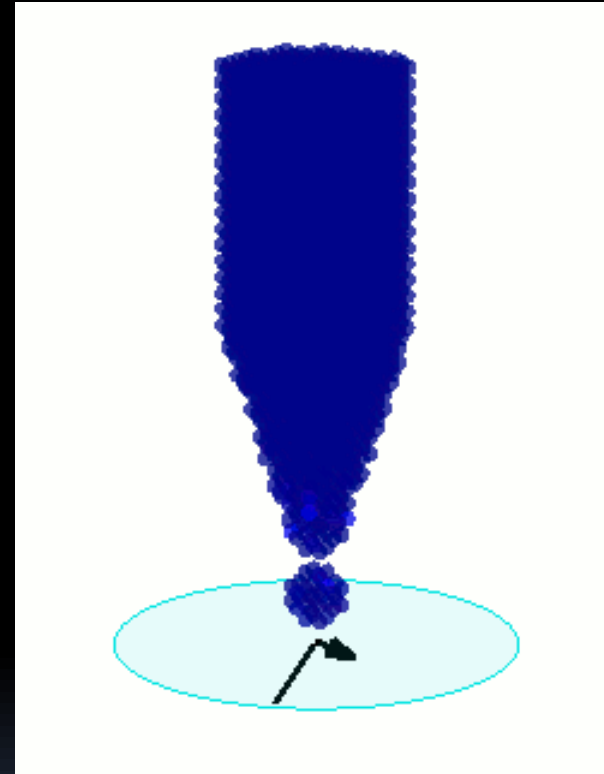


M. A.Taubenblatt and T. K.Tran, "Calculation of light scattering from particles and structures on a surface by the coupled-dipole method", J. Opt. Soc. Am. A, 10(5), (1993).

# DDI-SI: TM VS TE COUPLING



TM incident

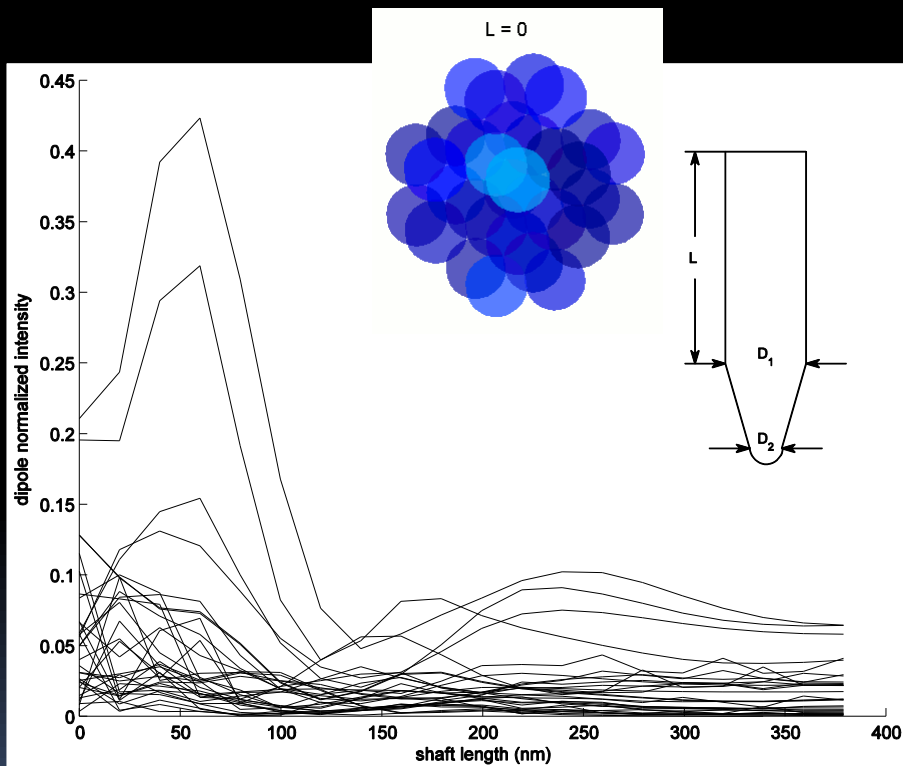


TE incident

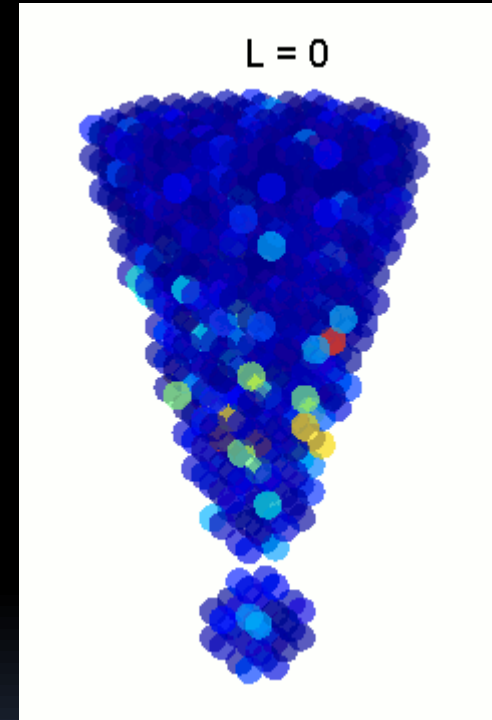
$$\lambda = 632\text{nm}$$

# AFM PROBE SHAFT LENGTH

- Field intensity of the 32 dipoles in the nanoparticle

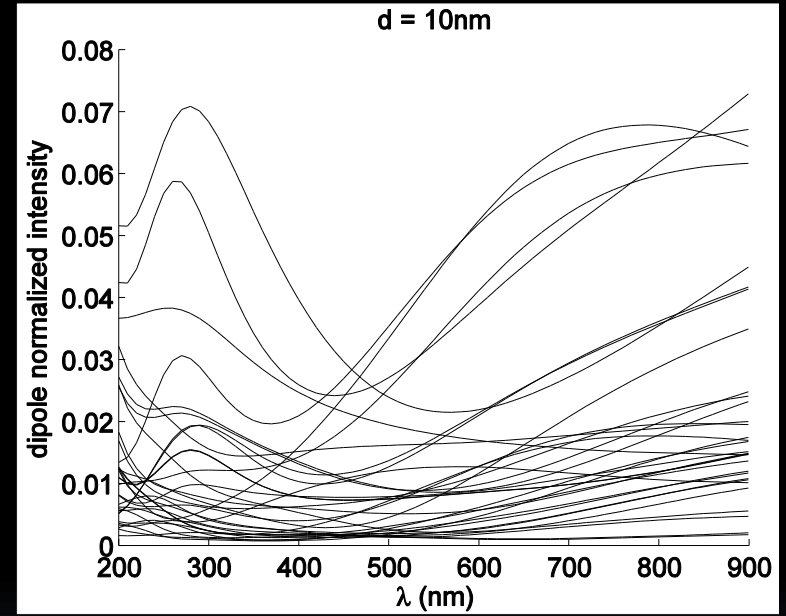
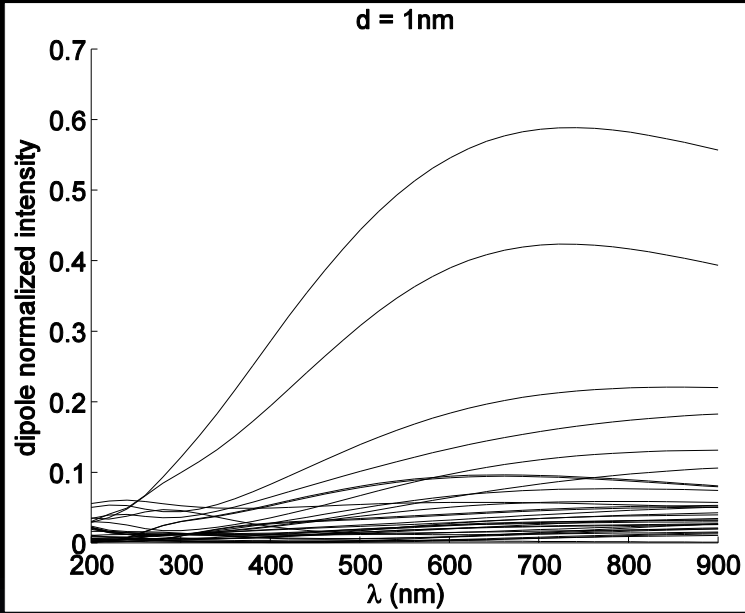


TM incident,  $\lambda = 632\text{nm}$





# Wavelength

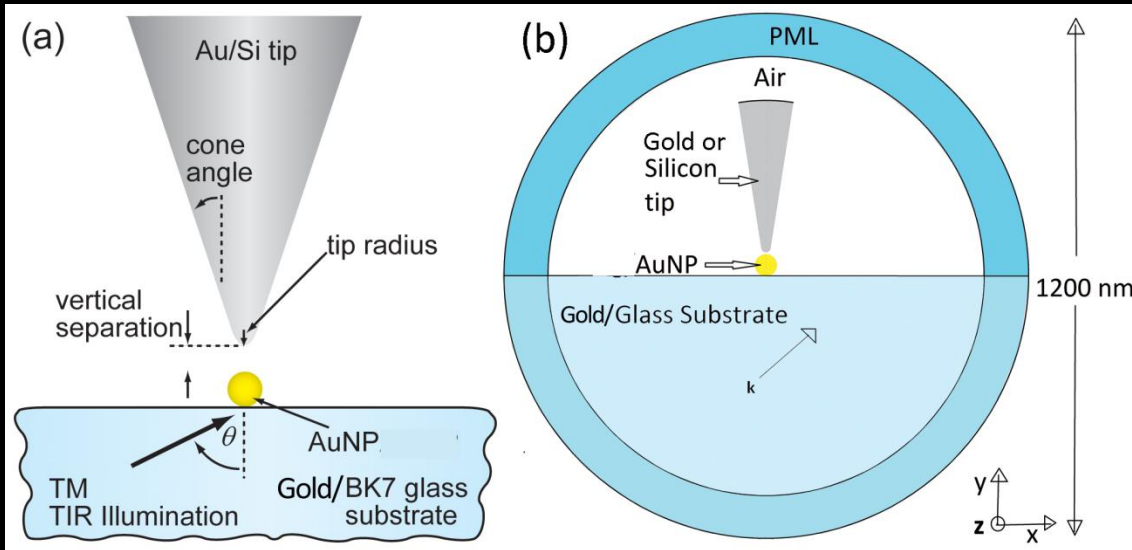


# Conclusion

- DDA-SI is a useful tool for studying near-field coupling for systems comprising nano-objects on or in the vicinity of a substrate
- It currently does not account for emission
- We can calculate optical forces
- Half-space T-matrix for system can be formulated
- Arbitrarily complex configurations are limited by available memory
- Irregular local area for substrate possible

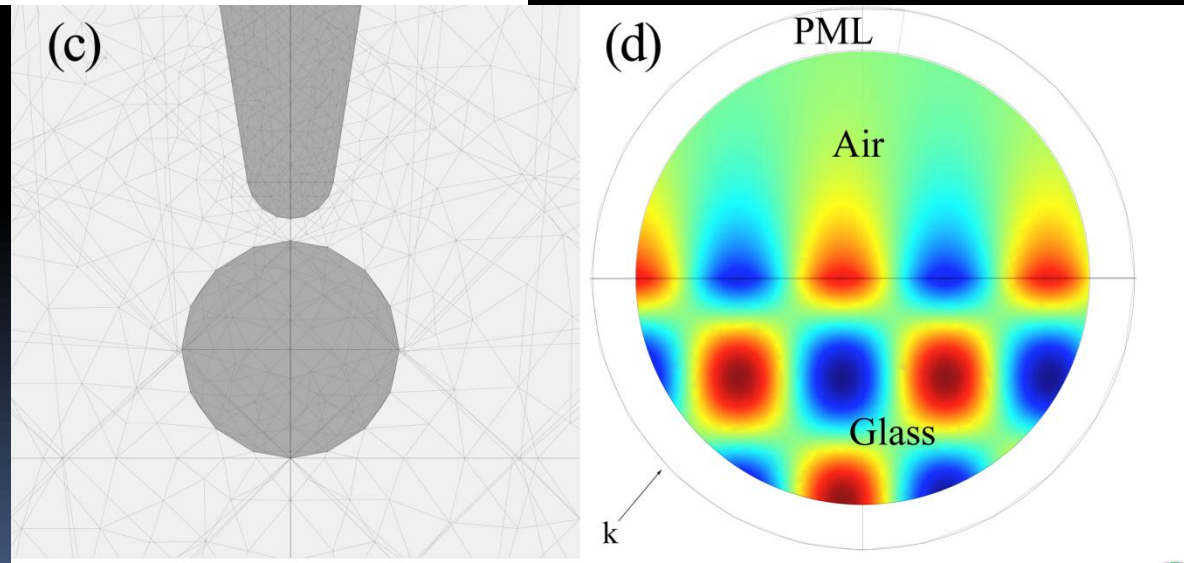
# NUMERICAL MODELING OF AFM-BASED MANUFACTURING

# Nano-Scale Patterning via AFM: (Gazi Huda)



- Spherical simulation domain
- Symmetric plane

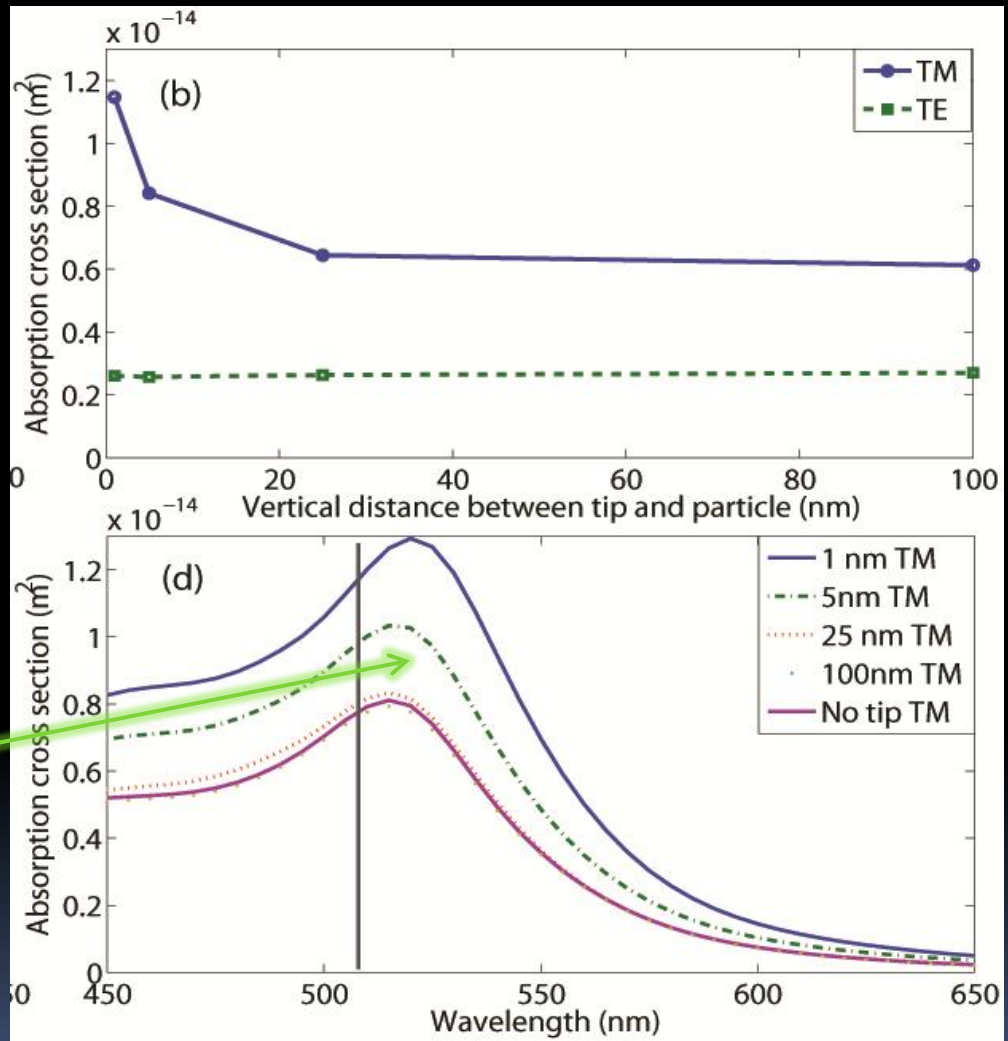
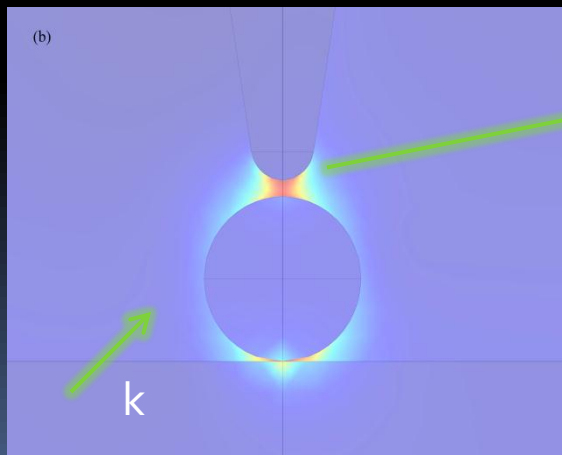
- Field defined analytically everywhere, except PML
- Setup checked with known solutions, and tested for convergence



# Effect of the Tip on Particle Absorption (TM)

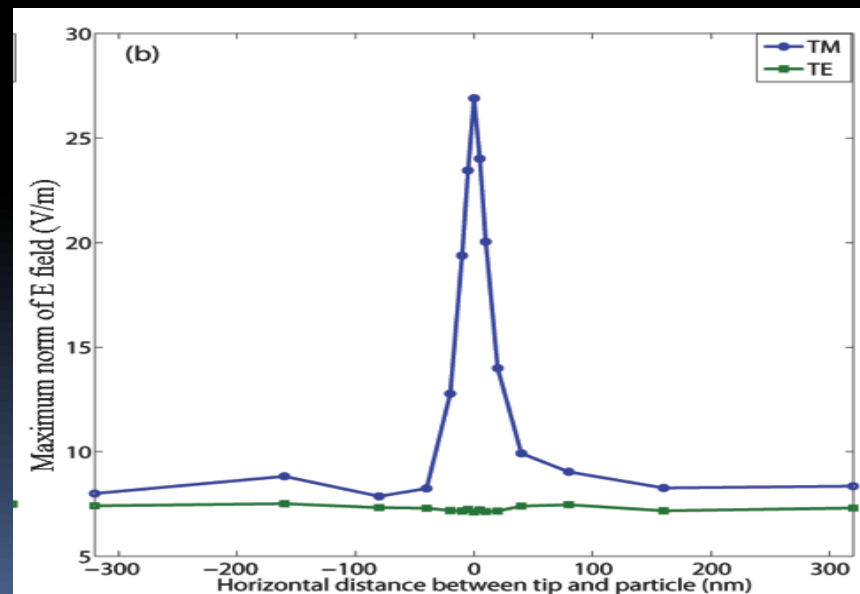
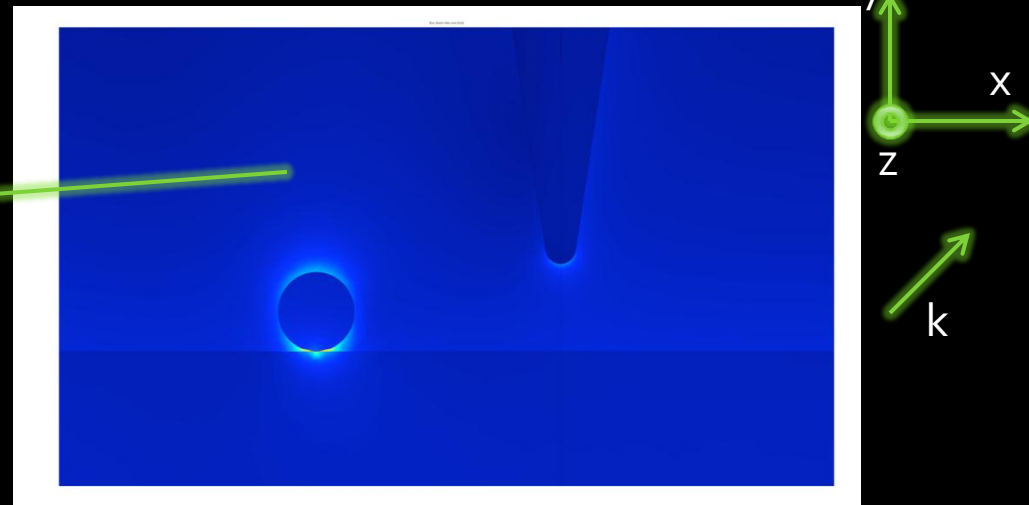
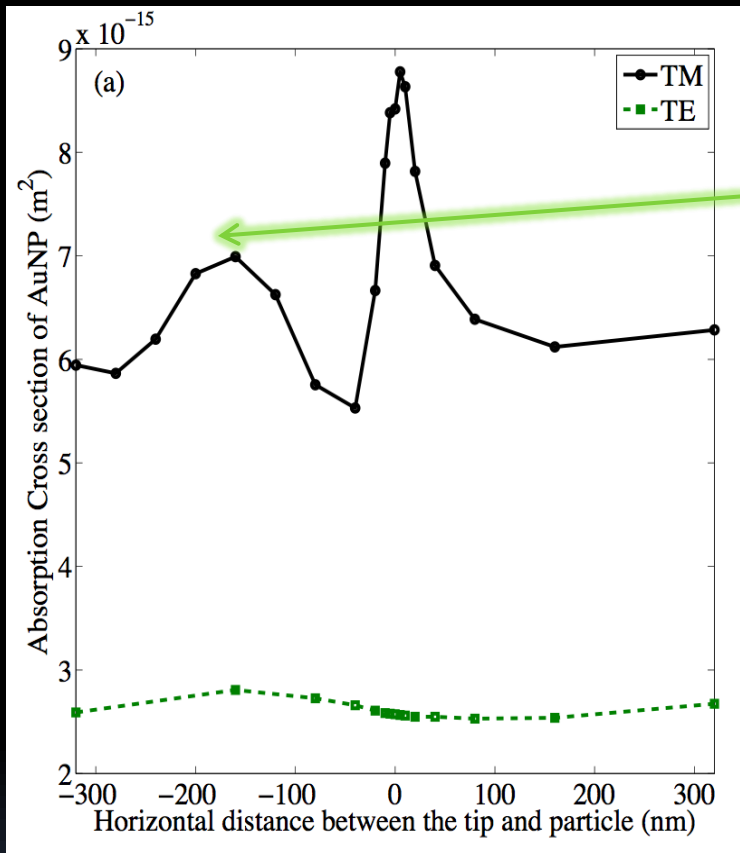
As tip is brought closer to particle:

- Absorption enhances.
- Resonant wavelengths get red shifted.
- Quantum effects were not taken into account.

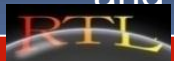


Huda, Hastings, Menguc et al. *Opt. Express* 2011

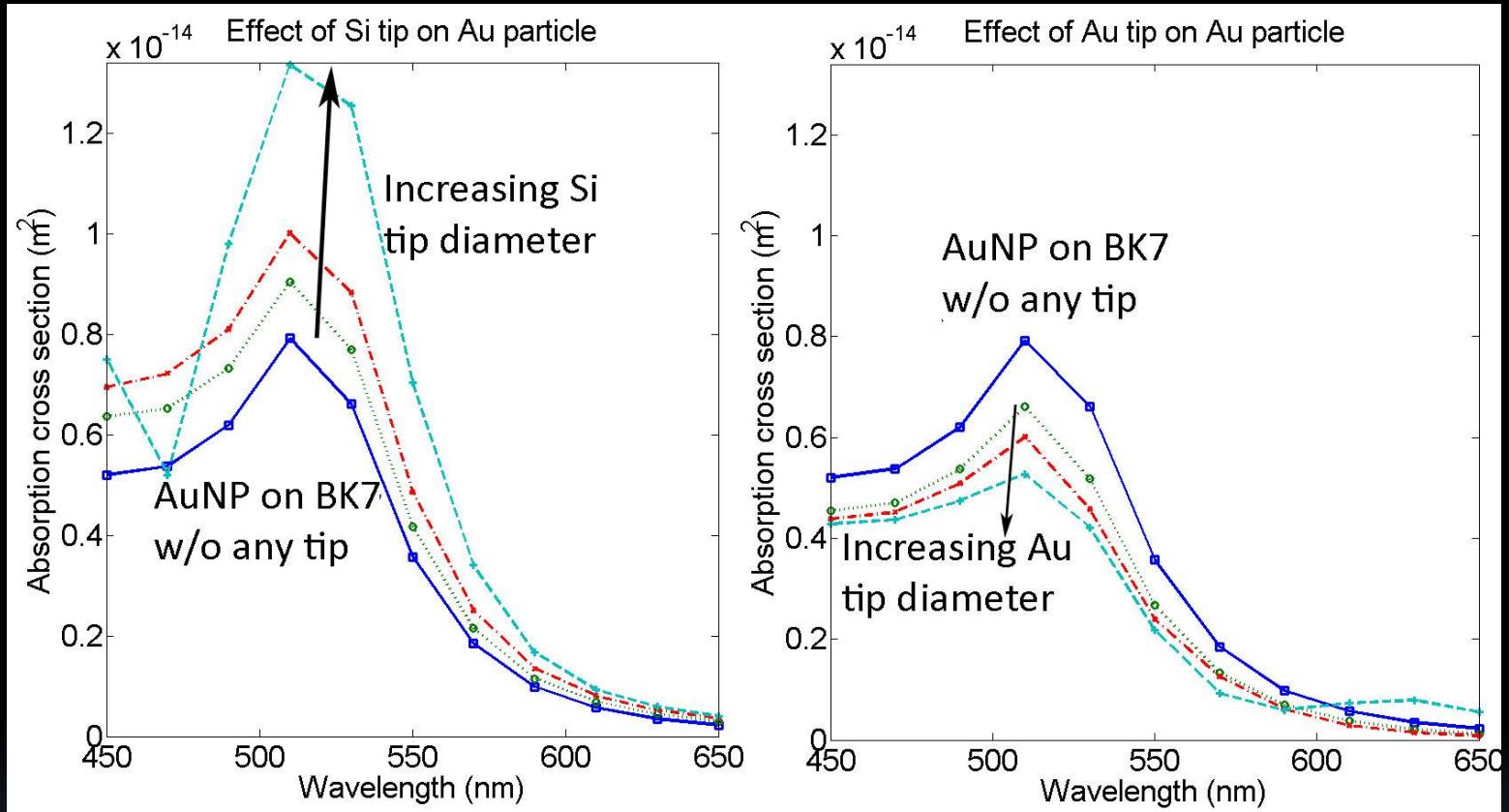
# Preliminary results: Effect of Tip on Particle Absorption w.r.t. Lateral Separation (TM & TE)



- highest absorption when particle 5 nm right of tip.
- Secondary peak might be because of the interference between the particle and tip.



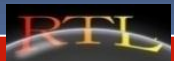
# Absorption modification caused by a tip



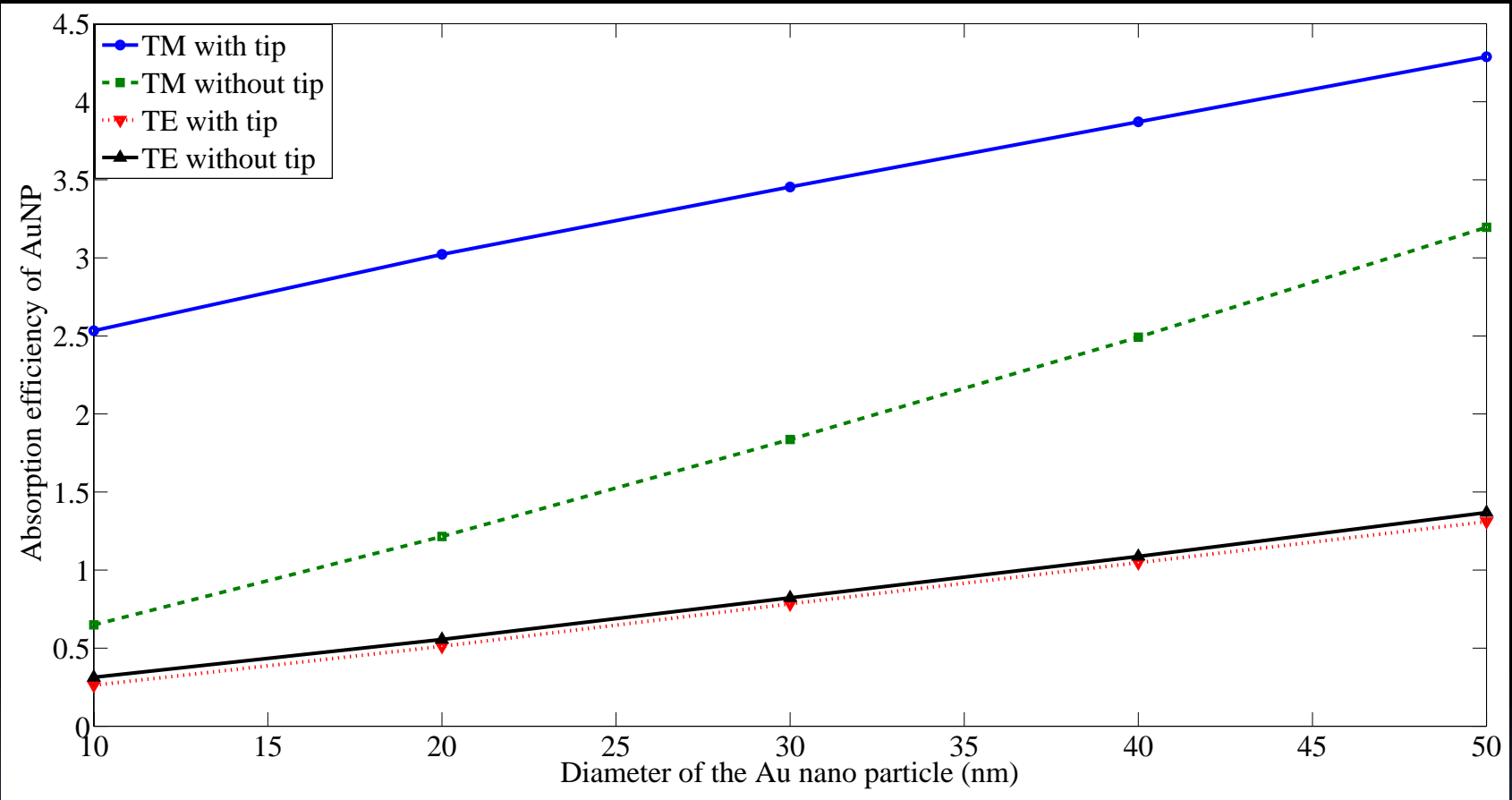
At total internal reflection illumination

- The field is strongly localized and enhanced under a nanoscale tip
- The absorption is enhanced under a Si tip
- The absorption is suppressed under a Au tip.

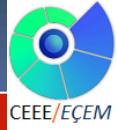
Huda et al. *IEEE JSTQE Nanoplasmonics* 2013



# Effect of tip on different particle size



Efficiency=Cross section/geometrical cross sectional area  
Greatest enhancement is when radius of particle is smaller than the tip



# THE STORY: NANO- & CASCADED PV & TPV

US 20100031990A1

(19) **United States**

(12) **Patent Application Publication**

**Francoeur et al.**

(10) **Pub. No.: US 2010/0031990 A1**

(43) **Pub. Date: Feb. 11, 2010**

(54) **CASCADED PHOTOVOLTAIC AND THERMOPHOTOVOLTAIC ENERGY CONVERSION APPARATUS WITH NEAR-FIELD RADIATION TRANSFER ENHANCEMENT AT NANOSCALE GAPS**

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(21) Appl. No.: **12/534,322**

(22) Filed: **Aug. 3, 2009**

#### Related U.S. Application Data

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#### Publication Classification

(51) **Int. Cl.**  
**H01L 35/00** (2006.01)  
**H01L 21/50** (2006.01)  
(52) **U.S. Cl.** ..... **136/206; 438/55; 257/E21.499**

#### (57) **ABSTRACT**

A cascaded photovoltaic/thermophotovoltaic energy conversion apparatus, a cascaded thermophotovoltaic energy conversion apparatus, and a method for forming the apparatuses are provided. The cascaded photovoltaic/thermophotovoltaic apparatus includes a photovoltaic device that receives solar radiation on an upper surface thereof and produces a first electric current output and a thermal radiation output, and a thermophotovoltaic device disposed a predetermined distance below a lower surface of the photovoltaic device, the thermophotovoltaic device receiving the thermal radiation output and converting the received thermal radiation output into a second electric current output. The cascaded thermophotovoltaic apparatus includes a radiator maintained at constant temperature via an external heat input on its upper surface and produces a thermal radiation output, and a thermophotovoltaic device disposed a predetermined distance below a lower surface of the radiator, the thermophotovoltaic device receiving the thermal radiation output and converting the received thermal radiation output into a first electric current output.

# ACKNOWLEDGMENTS

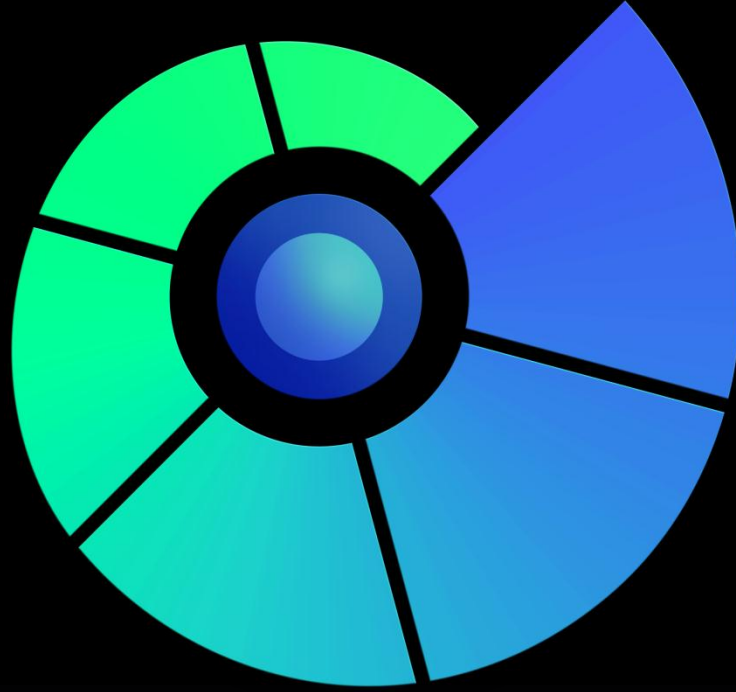
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