

Epsilon-Near-Zero behavior from Plasmonic Dirac Point: Theory and realization using 2D materials

Marios Mattheakis

Collaborators:

C. Valagiannopoulos
E. Kaxiras

School of Engineering &
Applied Physics (SEAS)

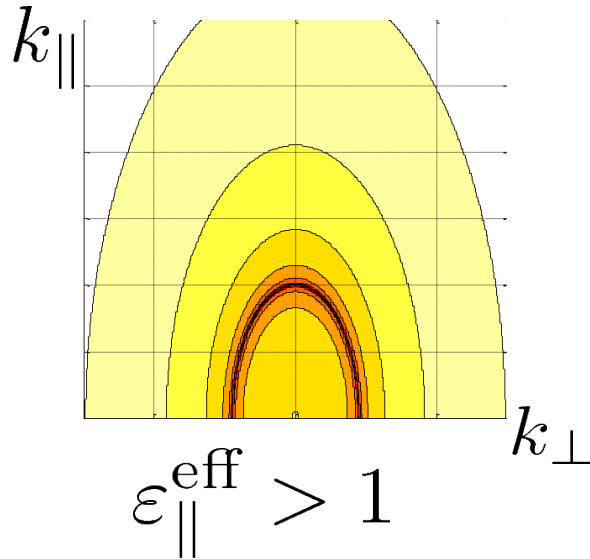
**APS March Meeting,
March 13, 2017
New Orleans, Louisiana**



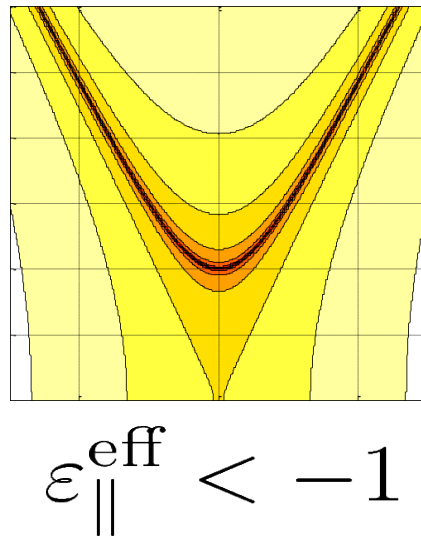
Periodic Structures

Plasmonic Crystal: Periodic arrangement of dielectric/metal slabs

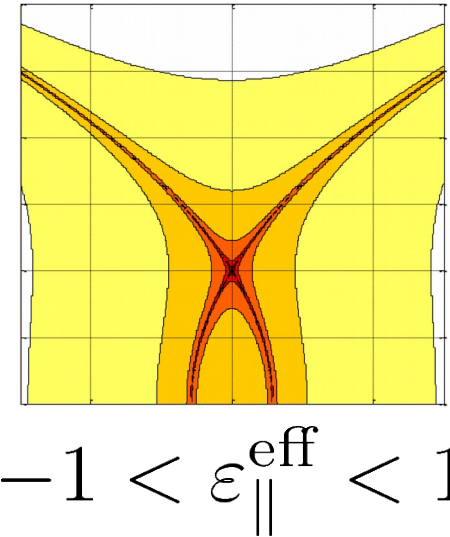
Optical Bands: The propagation modes form bands in k-space



Normal Refraction



Negative Refraction



Epsilon-Near-Zero (ENZ)

Motivation

Can we design a structure with **dynamically tunable** optical bands?

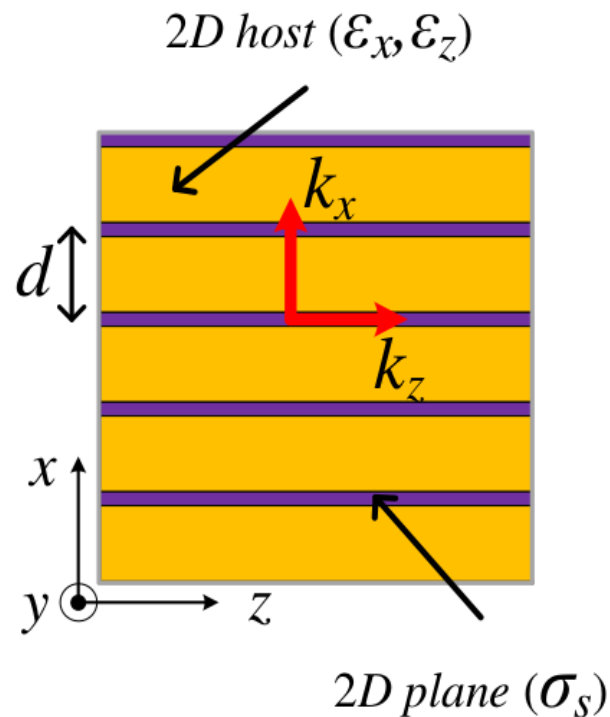
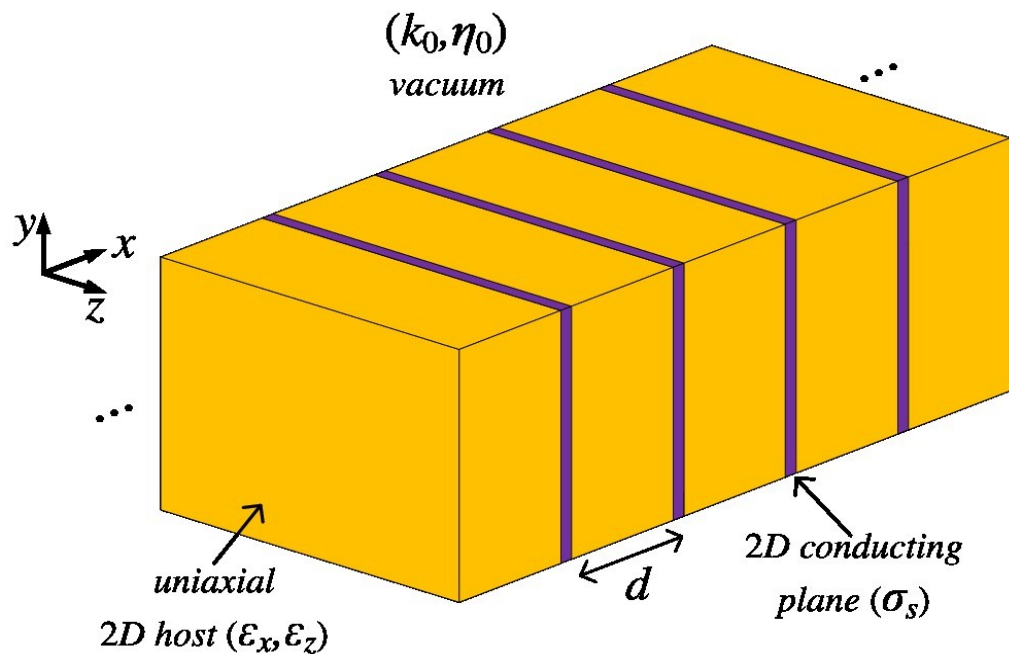
Can we have **ENZ behavior** between normal and negative refraction regimes?

What the **shape of ENZ band** will be?



Structure

2D metals are embedded periodically in an anisotropic dielectric host



Maxwell Equations

Transverse Magnetic (TM) monochromatic EM waves

$$-i\frac{\partial}{\partial z}\Psi = \mathcal{M} \cdot \Psi \Leftrightarrow$$
$$-i\frac{\partial}{\partial z} \begin{pmatrix} E_x \\ H_y \end{pmatrix} = k_0\eta_0 \begin{pmatrix} 0 & 1 + \frac{1}{k_0^2} \frac{\partial}{\partial x} \frac{1}{\epsilon_z} \frac{\partial}{\partial x} \\ \frac{\epsilon_x}{\eta_0^2} & 0 \end{pmatrix} \begin{pmatrix} E_x \\ H_y \end{pmatrix}.$$
$$E_z = \frac{i\eta_0}{k_0\epsilon_z} \frac{\partial H_y}{\partial x}$$

EigenValue Problem

$$\Psi(x, z) = \Psi(x)e^{ik_z z}$$

$$k_z \Psi = \mathcal{M} \Psi$$



Dispersion Relation

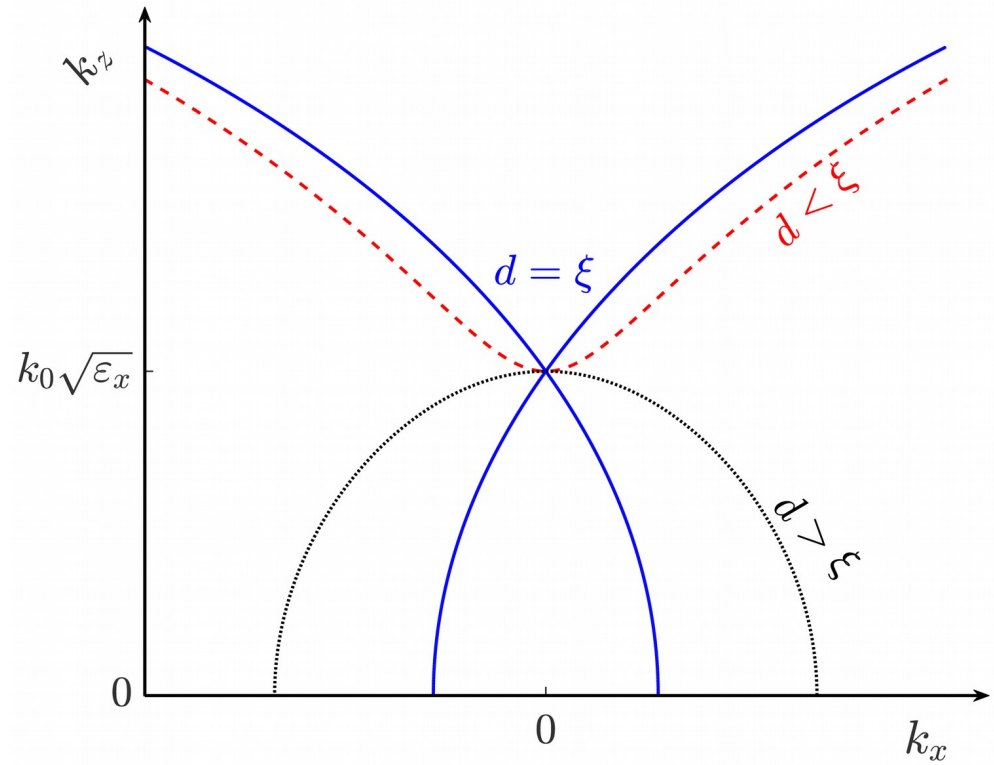
Dense grid $\lambda \gg d$:

$$\frac{k_z^2}{\epsilon_x} + \frac{d}{(d - \xi)\epsilon_z} k_x^2 = k_0^2$$

Plasmonic Thickness

$$\xi = -\frac{i\sigma_s\eta_0}{k_0\epsilon_z} = 2\delta$$

(B.Wang et. al. PRL 109, 2012)



Plasmonic Dirac Point (PDP)



A Plasmonic Dirac Point leads to ENZ

Effective medium (metamaterial) approach

$$\epsilon_z^{\text{eff}} = \epsilon_z \frac{d - \xi}{d}, \quad \epsilon_x^{\text{eff}} = \epsilon_x$$

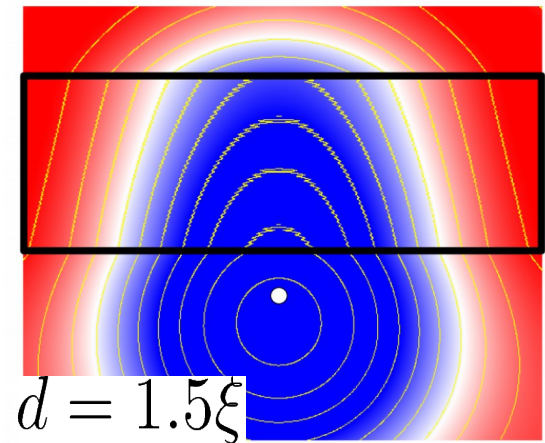
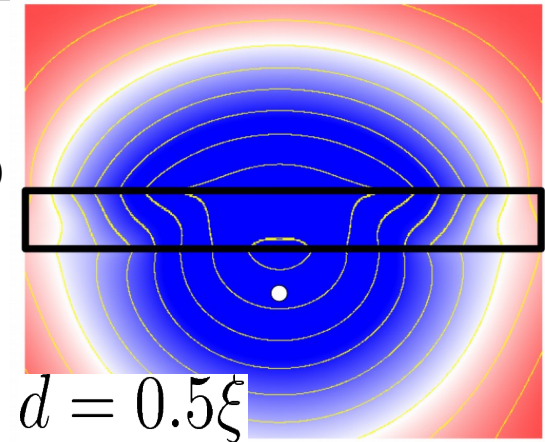
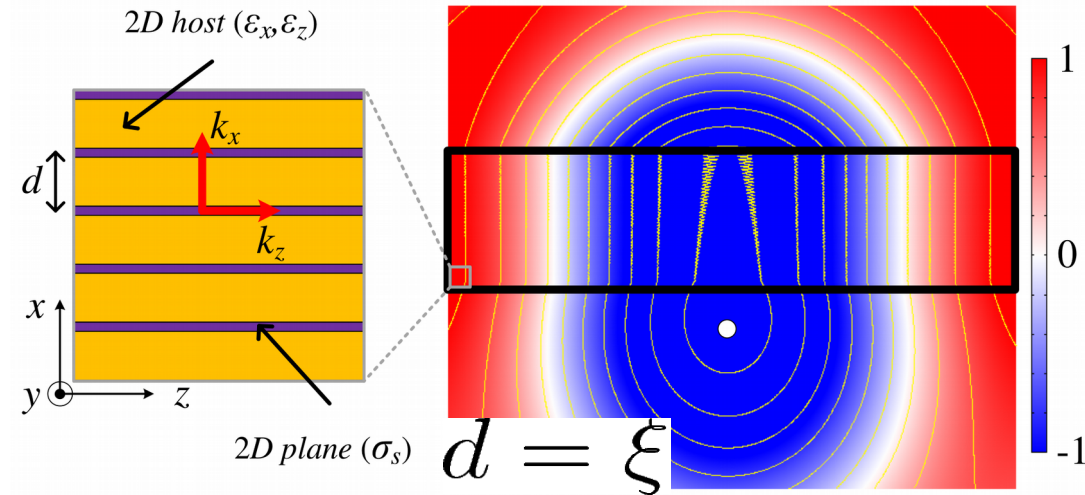
Plasmonic Dirac Point leads to Epsilon-Near-Zero behavior

$$d = \xi \Rightarrow \epsilon_z^{\text{eff}} = 0$$



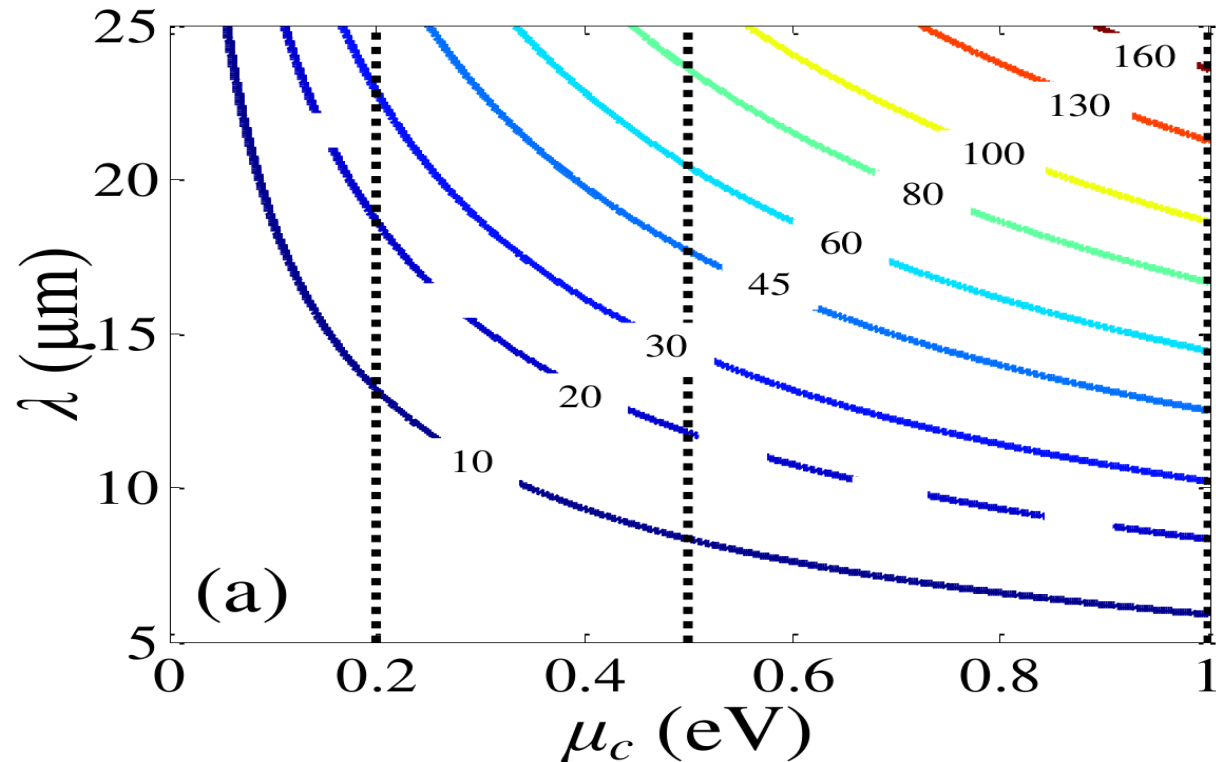
EM wave simulations

- 40 periods structure: doped graphene layers embedded in MoS₂ host ($\epsilon_x=3.5$, $\epsilon_z=13$)
(R.K. Defo *et. al.* PRB **94**, 2016)
- 2D magnetic dipole source
- $\lambda_0 = 12 \mu\text{m}$ ($f = 25 \text{ THz}$), $\xi=20.8 \text{ nm}$



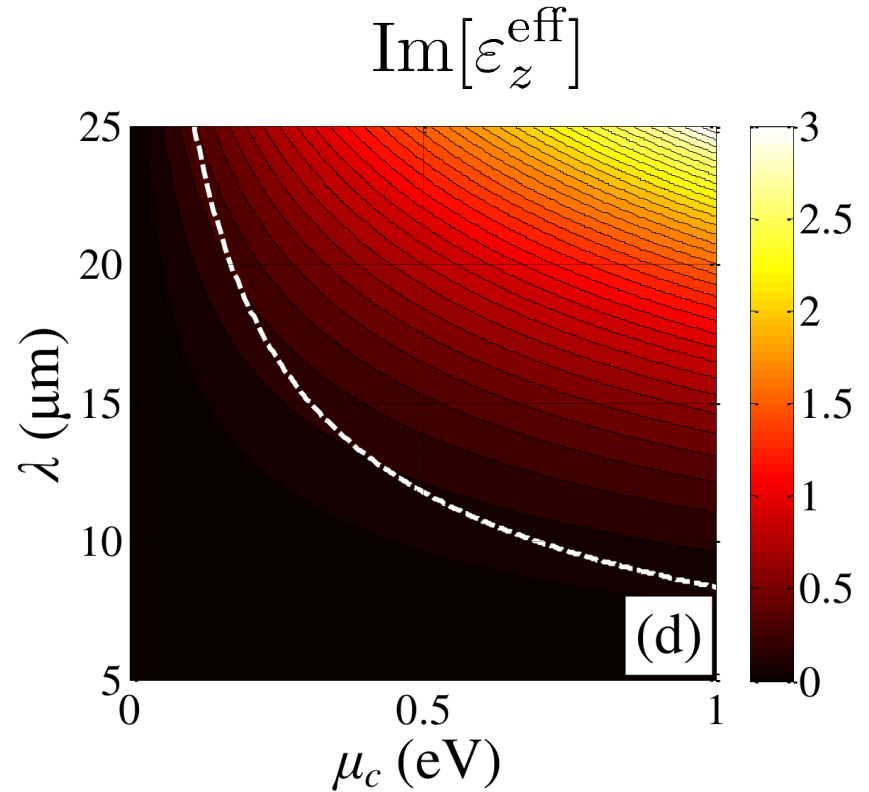
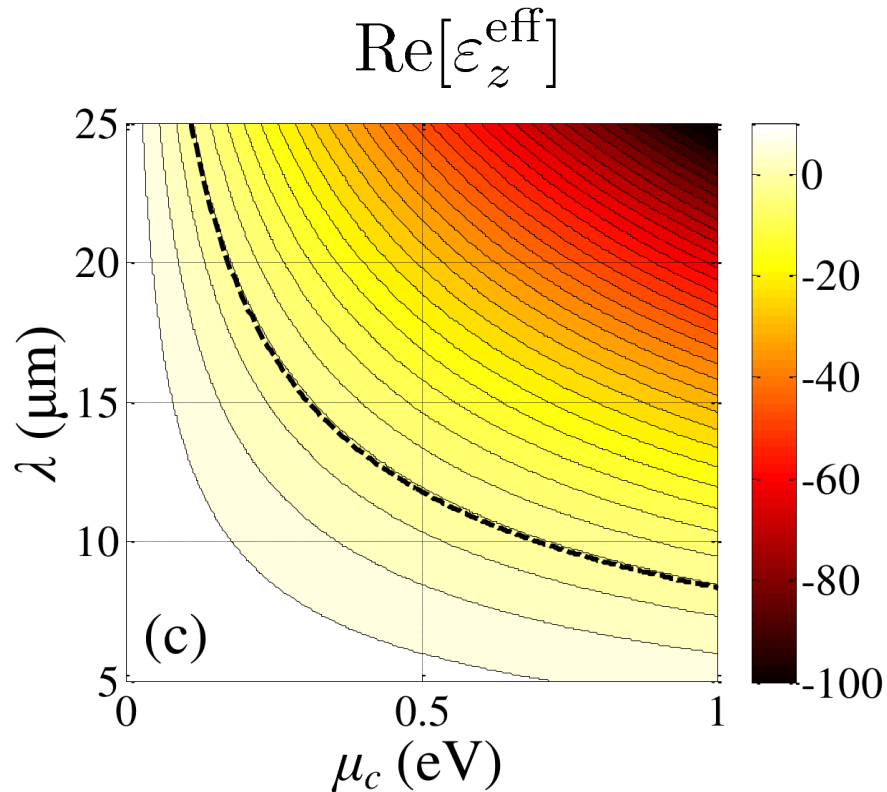
Tunability in terms of λ , μ_c & d

Combinations of μ_c and λ leading to PDP & ENZ (d is plotted in nm).



Effective Permittivity

Combinations of λ and μ_c at fixed period $d=20\text{nm}$. Dashed lines indicate ENZ regime.



Conclusion

- Any periodic structure of 2D plasmonic materials (e.g. doped graphene) exhibits Plasmonic Dirac Point in k-space.
- A Plasmonic Dirac Point leads to **Epsilon-Near-Zero** metamaterial.
 - ✓ A systematic method for designing ENZ metamaterials.
- Optical properties can be tuned dynamically via doping and frequency.
 - ✓ Tunable Metamaterial.

Relevant Publication:

M. Mattheakis, C.A. Valagianopoulos and E. Kaxiras, Phys. Rev. B, **94**, 201404(R), 2016.



Acknowledgment

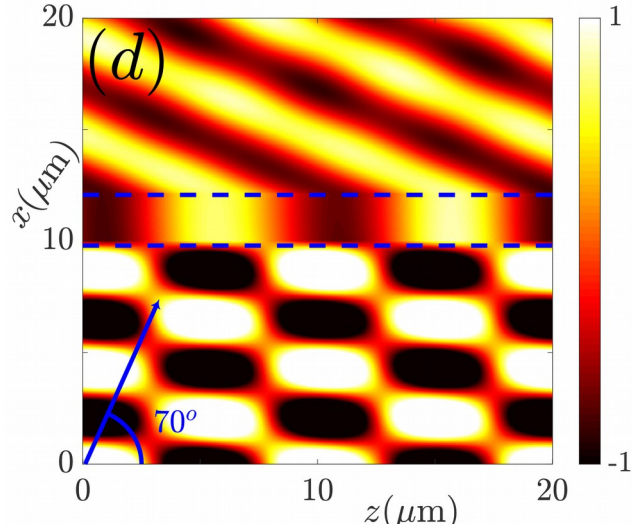


ODYSSEY
HARVARD FAS
RESEARCH COMPUTING

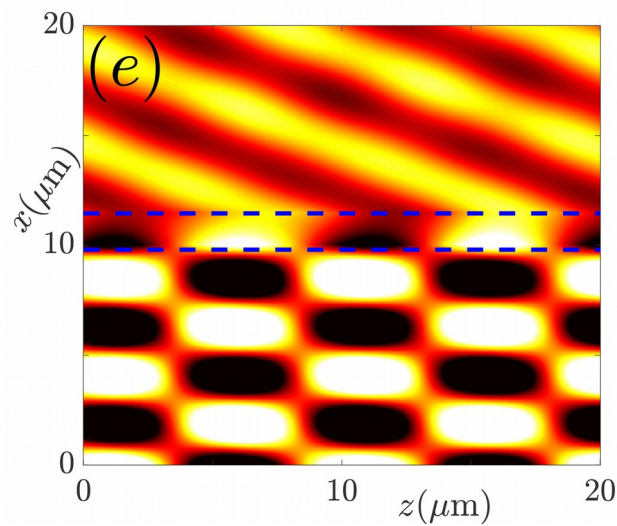


Plasmonic Metamaterial (simulations)

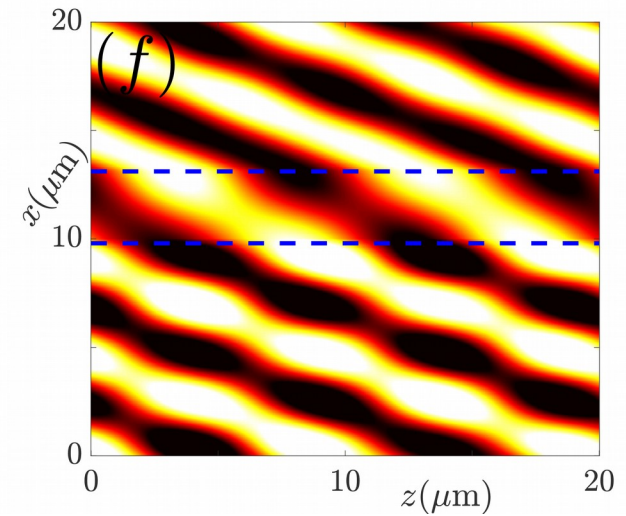
100 periods structure is excited by a plane wave source of $f=25$ THz
($\lambda=12\mu\text{m}$).



$d=\xi=20,8$ nm (linear)



$d<\xi$ (hyperbolic)



$d>\xi$ (elliptic)

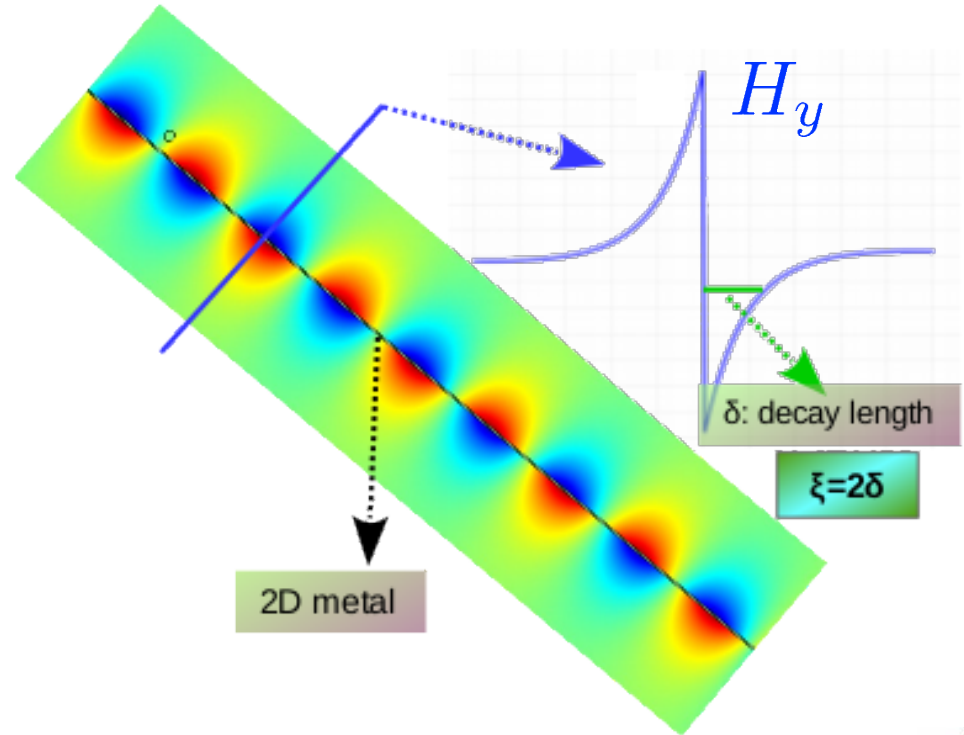
Dispersion Relation

Assuming a very dense grid $\lambda \gg d$:

$$\frac{k_z^2}{\epsilon_x} + \frac{d}{(d - \xi)\epsilon_z} k_x^2 = k_0^2$$

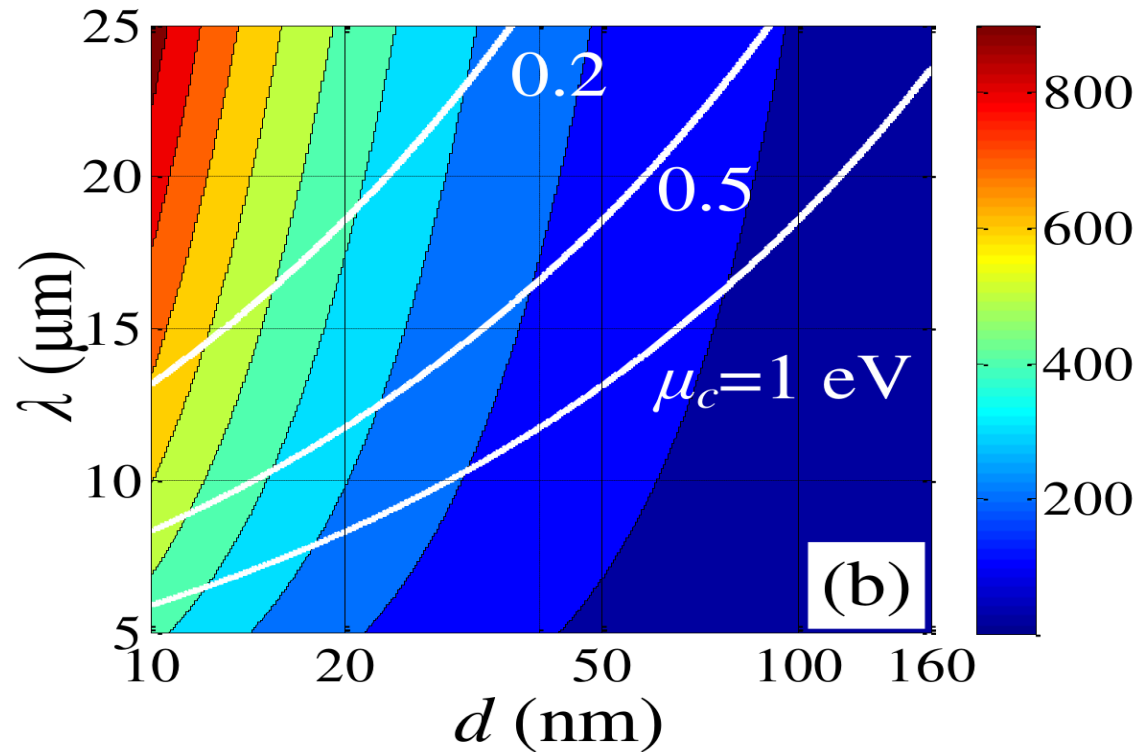
Plasmonic Thickness

$$\xi = -\frac{i\sigma_s\eta_0}{k_0\epsilon_z}$$



Propagation Length

Propagation length L/d for combinations of λ , d & μ_c leading to ENZ.



Plasmonic Metamaterial

Doped graphene surface conductivity:

$$\sigma_s = \frac{ie^2\mu_c}{\pi\hbar^2(\omega + i/\tau)} \quad (\tau = 0.5ps)$$

PDP is extremely sensitive to structural defects:

$$\frac{\Delta k_z}{k_0\sqrt{\epsilon_x}} = -\frac{6}{(k_0d)^2\epsilon_z} \frac{\Delta\xi}{d}$$

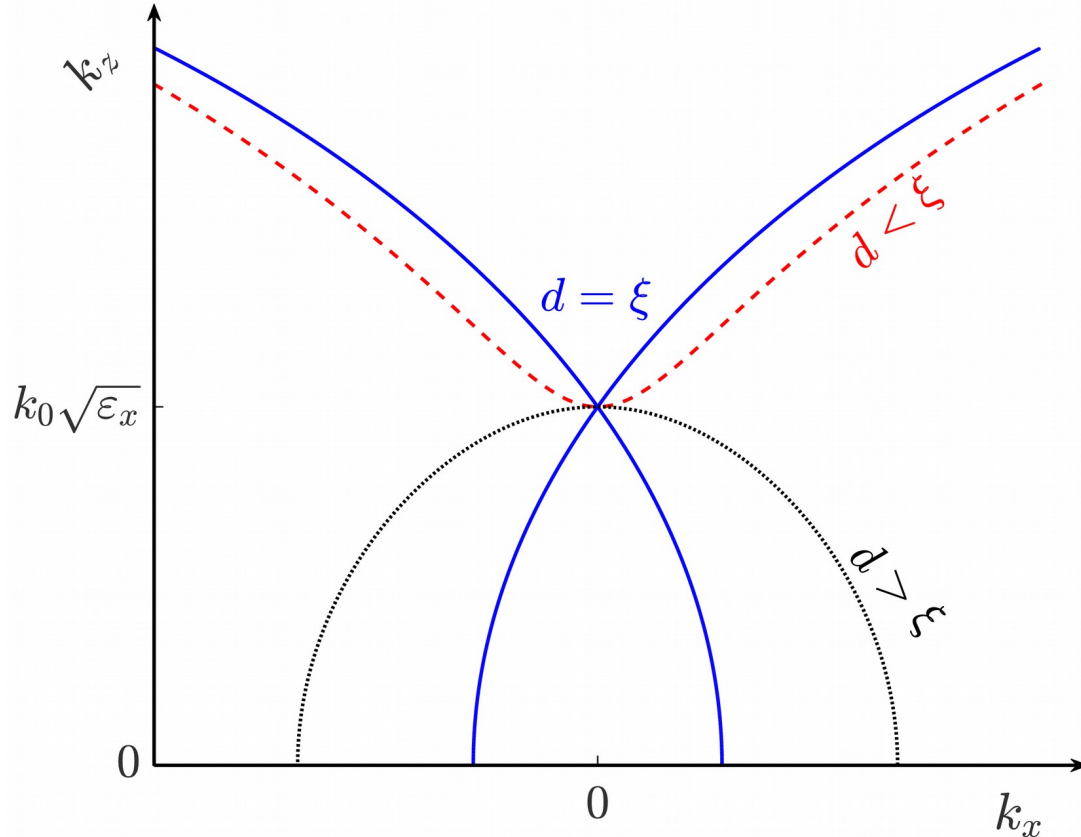
Stacking of 2D materials provides essentially perfect planarity.

Stacking of MoS2 builds a anisotropic dielectric:

$$\epsilon_x = 3.5 \quad , \quad \epsilon_y = \epsilon_z = 13 \quad (\text{R.K. Defo et. al. PRB } \mathbf{94}, 2016)$$



Optical Bands



Weak plasmon coupling

Strong plasmon coupling

Critical plasmon coupling

Plasmonic Dirac Point (PDP)

$$k_z^2 \approx \frac{\epsilon_x d}{\epsilon_z (\xi - d)} k_x^2$$

