

# Graphene epsilon-near-zero plasmonic crystals

Marios Mattheakis

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Dublin, Ireland

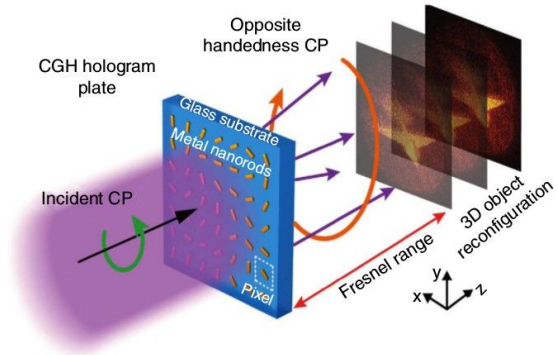


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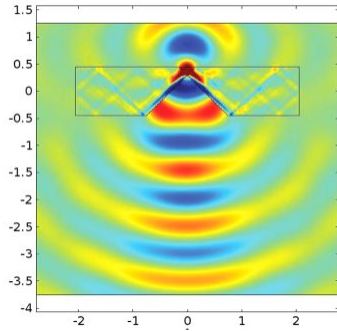


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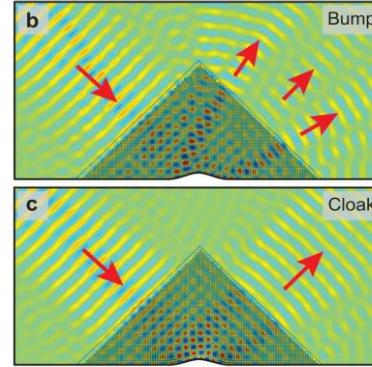
# Metamaterials



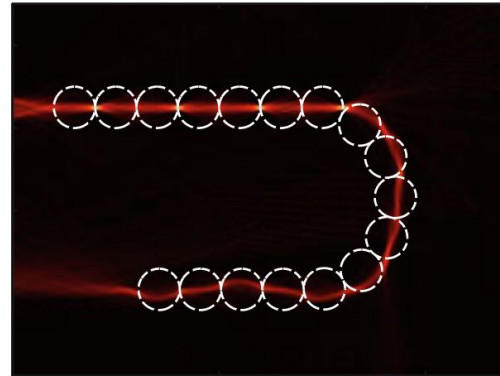
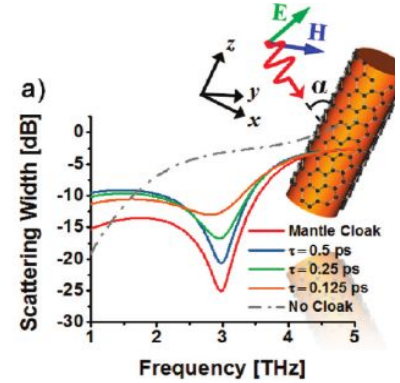
3D optical holography. Nat. Comm. **4** 2013



Hyperbolic antennas shape radiation pattern. JAP **116** 2014

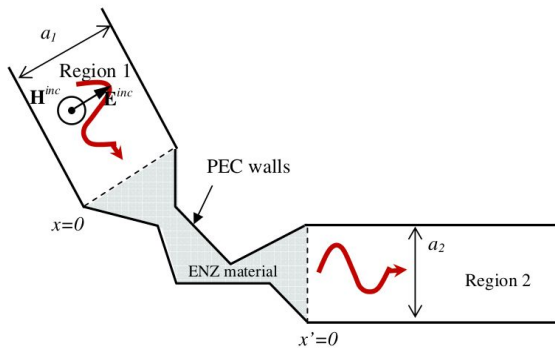


EM wave Cloaking. Sc. Rep. **78** 2011 & ACS Nano **7** 2011

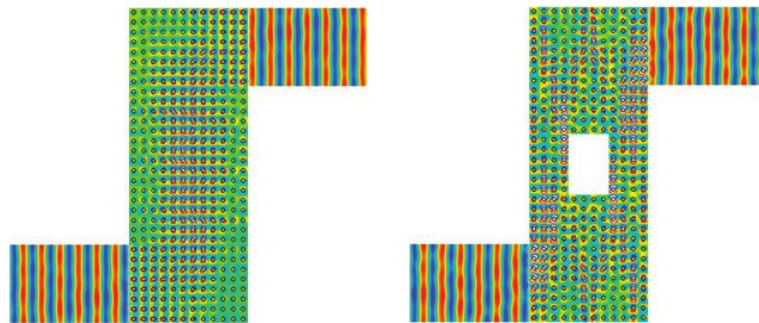


Efficient waveguides. J. Optics **14** 2012

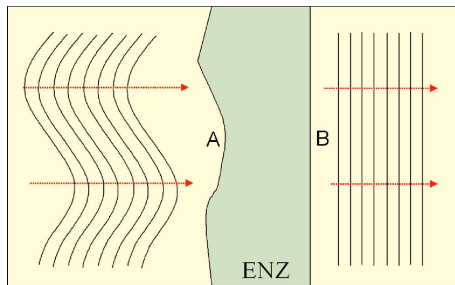
# Epsilon-Near-Zero (ENZ)



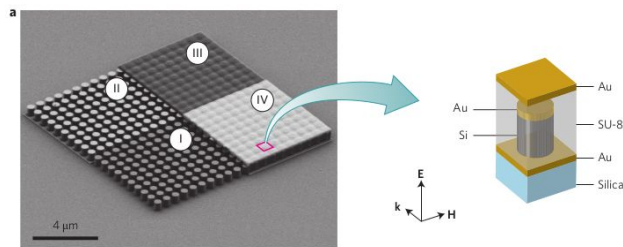
Tunneling through narrow channels. PRL **97** 2006



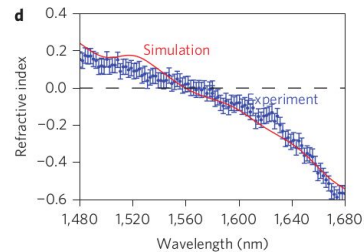
Bending and Cloaking. Nat. Mat. **10** 2011



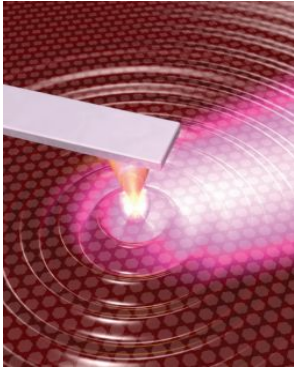
Tailoring the radiation phase pattern. PRB **75** 2007



On-chip zero-index. Nat. Phot. **9** 2015

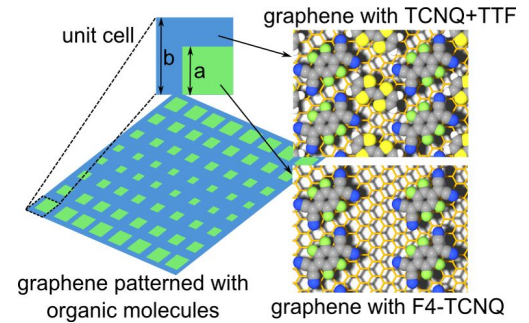


# Plasmons in two-dimensional materials

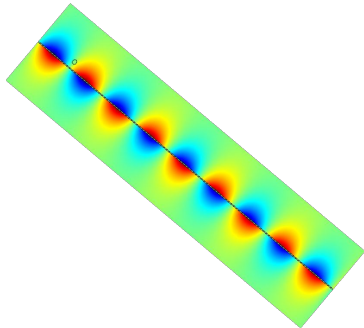


## Graphene, a semi-metal:

- Becomes metal after doping
- Large electrical conductivity
- Tunable conductivity via doping
- Reduced dimensions
- Low optical losses



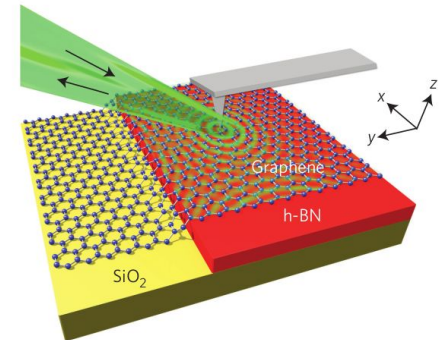
Nanoscale organic meta-lens. Nano Lett. **14** 2014



## Graphene plasmonics:

- Plasmons are charge oscillations
- THz plasmons with tunable properties
- Ultra-subwavelength plasmons

Nat. Phot. **6** 2012



Tunable hyperbolic media. Nat. NanoTech. **10** 2015

# Outline

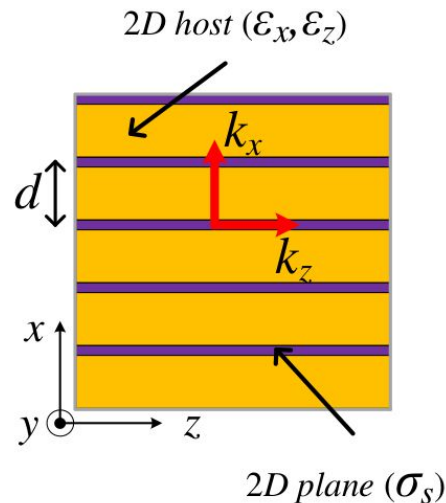
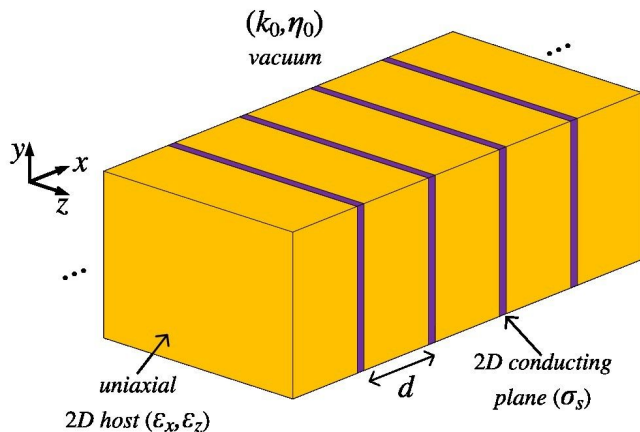
A systematic way to design ENZ plasmonic crystals based on two-dimensional metals.

ENZ appears as a Dirac (linear) dispersion in k-space

- Anisotropic dielectric host: ENZ condition
- Space-dependent host: Universality of ENZ and Dirac dispersion
- Frequency-dependent host: Extending the ENZ frequency window
- Effective permittivity for arbitrary plasmonic crystal of 2D metals

# Plasmonic Crystal

Periodic arrangement of dielectric/metal slabs



2D metals are embedded periodically in an anisotropic dielectric host

The metals carry surface current  $J = \sigma E_z$

## Motivation:

Can we design tunable metamaterials with desirable effective permittivity ?

# Maxwell Equations

## Transverse Magnetic (TM) polarization

### Transversal Field

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

### Longitudinal Field

$$E_z = \frac{i \eta_0}{k_0 \epsilon_z} \frac{\partial H_y}{\partial x}$$

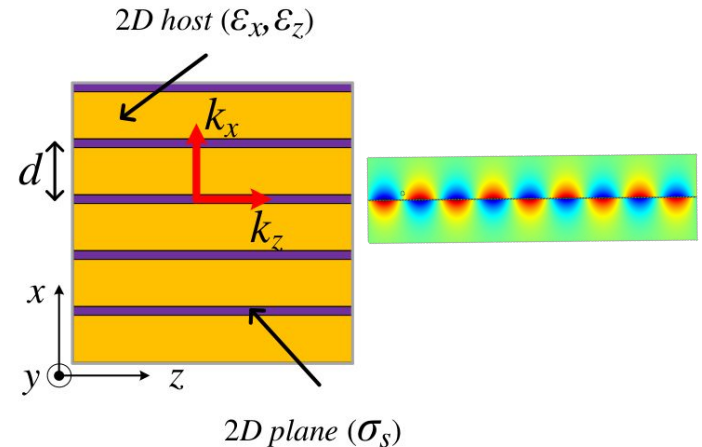
$$k_0 = \omega / c$$

$$\eta_0 = \sqrt{\mu_0 / \epsilon_0}$$

Propagation along z direction (plasmons)

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

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



# Dispersion Relation

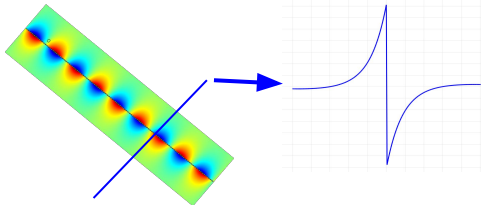
Assume periodicity along x direction (Bloch waves)

$$D(k_x, k_z) = \cos(k_x) - \left[ \cosh(\kappa d) - \frac{\xi d}{2} \sinh(\kappa d) \right] = 0$$

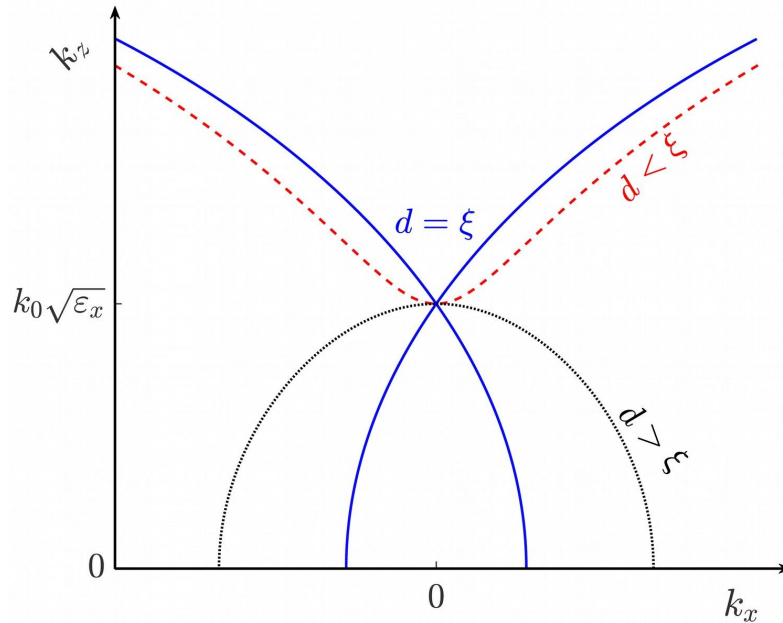
$$\kappa^2 = \frac{\epsilon_z}{\epsilon_x} (k_z^2 - k_0^2 \epsilon_x)$$

Plasmonic Thickness  
(twice the decay length)

$$\xi = -\frac{i\sigma}{\omega\epsilon_z}$$



Wang *et. al.* PRL **112** 2012



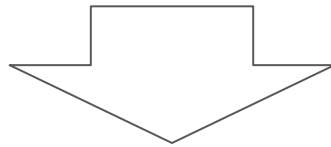
MM *et. al.* PRB **94** 2016



# Effective dielectric function

dense grid:  $d \ll \lambda$

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



effective medium

$$\frac{k_z^2}{\varepsilon_x^{\text{eff}}} + \frac{k_x^2}{\varepsilon_z^{\text{eff}}} = k_0^2$$

$$\varepsilon_z^{\text{eff}} = \frac{d - \xi}{d} \varepsilon_z$$

$$\varepsilon_x^{\text{eff}} = \varepsilon_x$$

ENZ condition

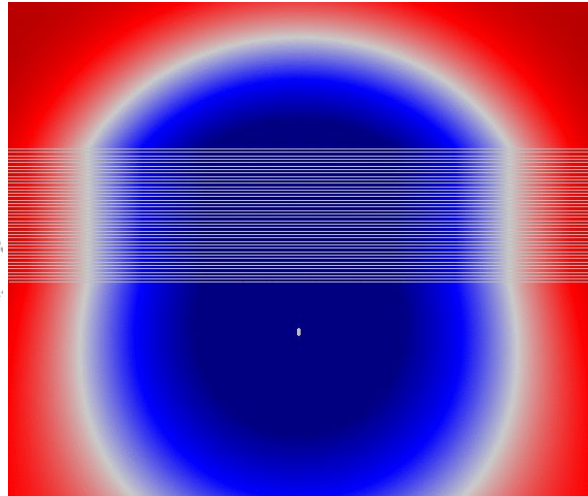
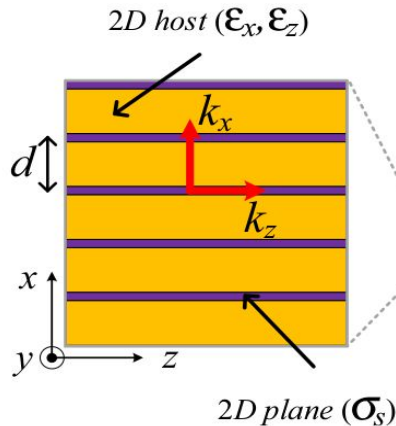
$$d = \xi \Rightarrow \varepsilon_z^{\text{eff}} = 0$$

- ✓ Dirac dispersion yields ENZ behavior
- ✓ Systematic method for designing ENZ metamaterials

# ENZ behavior (simulation)

- 40 graphene layers embedded in MoS<sub>2</sub> host ( $\epsilon_x=3.5$ ,  $\epsilon_z=13$ ,  $d=20.8$  nm).
- Drude model for graphene conductivity.
- $\lambda_0=12$   $\mu\text{m}$  (THz regime).
- 2D magnetic dipole source.

$$\sigma(\omega) = \frac{ie^2\mu_c}{\pi\hbar^2(\omega + i/\tau)}$$



Ultra fast phase transitions

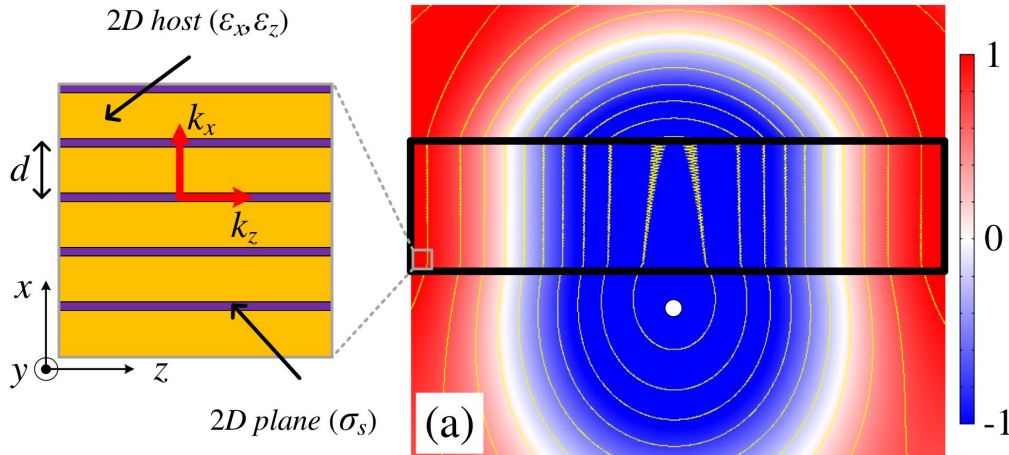
No dispersion

No phase delay

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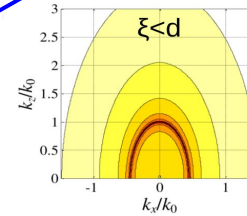
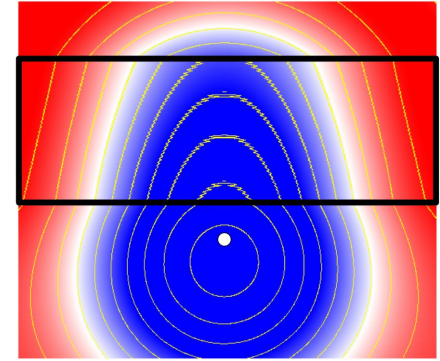
No phase delay

# Numerical EM wave simulations

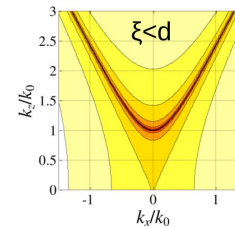
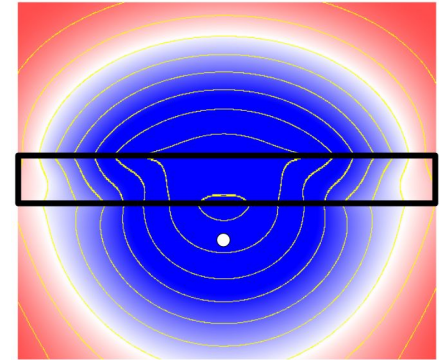
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COMSOL  
simulations

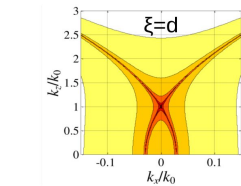
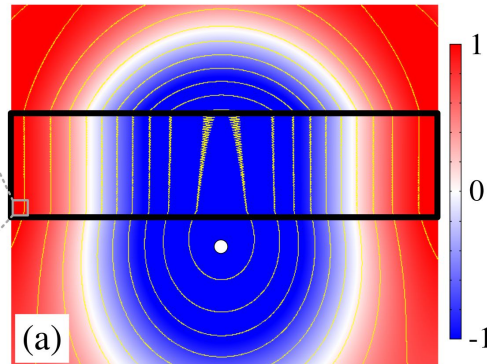
Weak plasmon coupling



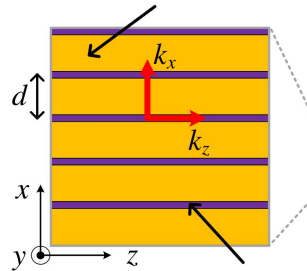
Strong plasmon coupling



Dirac Dispersion



2D host ( $\epsilon_x, \epsilon_z$ )



2D plane ( $\sigma_s$ )

(a)

# Outline

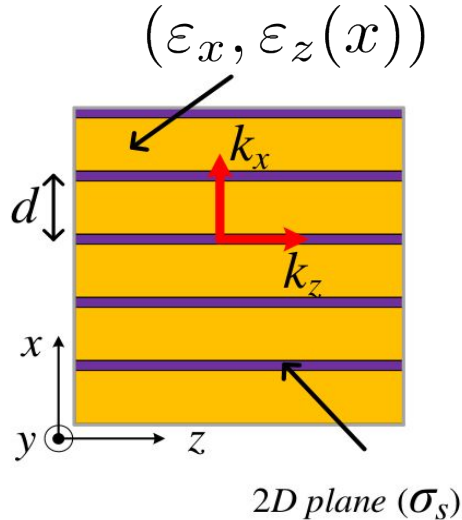
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# Universal behavior of a Dirac dispersion

Dirac dispersion and ENZ is a **universal property** of plasmonic crystals consisting of 2d metals in host with space-dependent permittivity



## Universal condition for ENZ

$$d_0 = \xi_0 \left[ \int_0^1 f(x) dx \right]^{-1}, \quad \frac{\epsilon_z^{\text{eff}}}{\epsilon_{z,0}} = \xi_0 \left( \frac{1}{d_0} - \frac{1}{d} \right)$$

$$\epsilon_z(x) = \epsilon_{z,0} f(x/d), \quad f(x) > 0$$

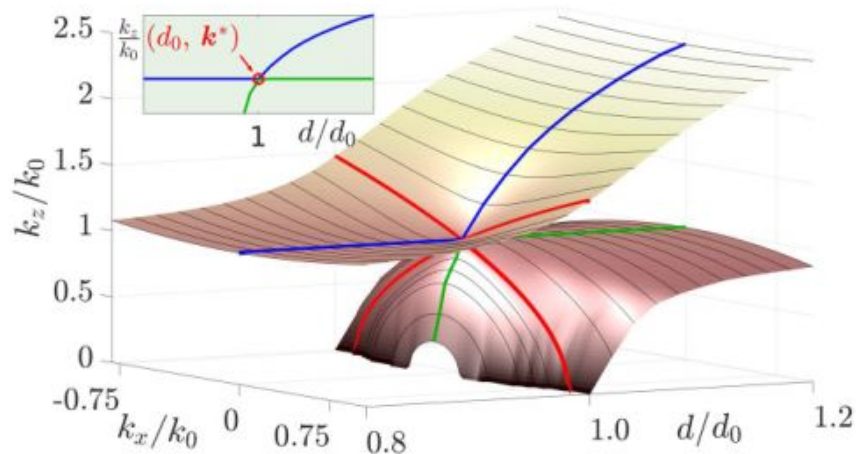
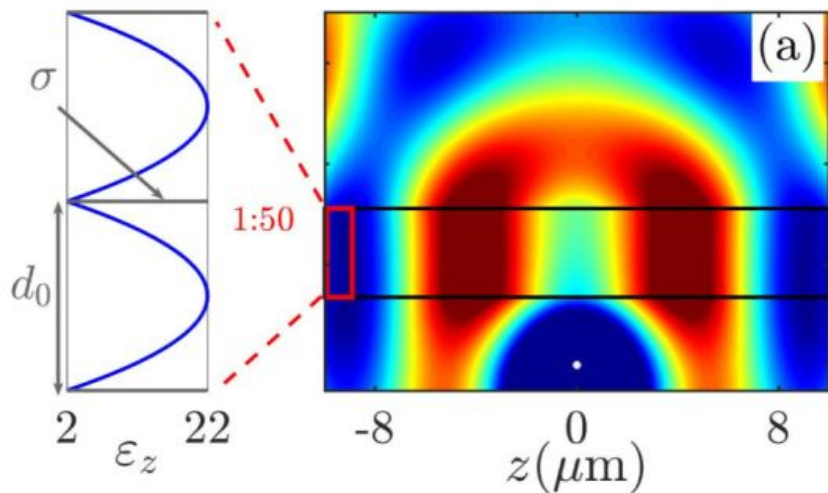
$$\xi_0 = -\frac{i\sigma}{\omega\epsilon_{z,0}}$$

Introduce an extra degree of freedom for tuning the dielectric properties

# Universal behavior of a dispersive Dirac cone

Parabolic profile

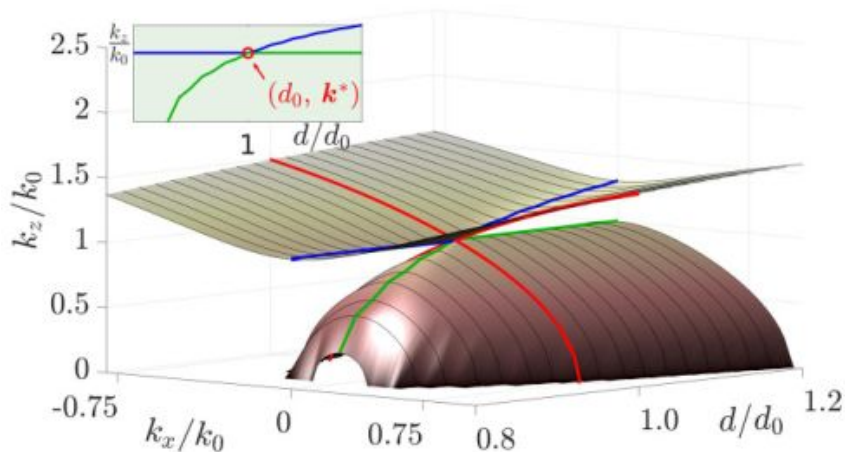
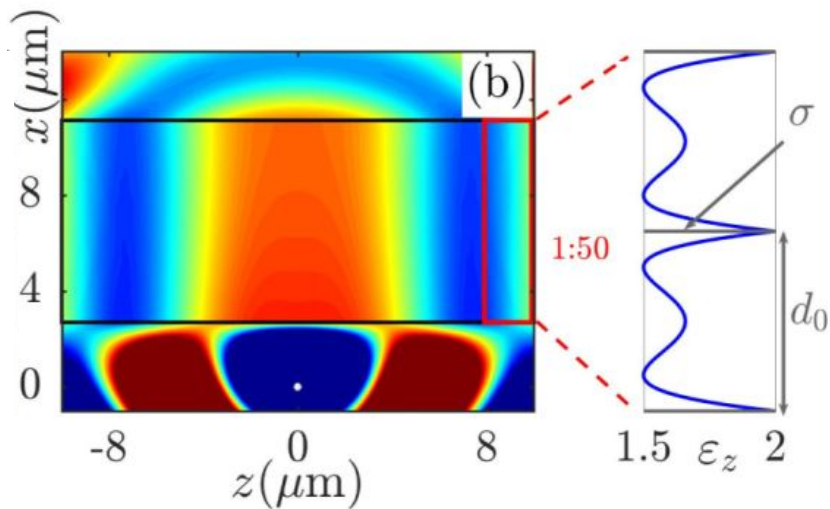
$$\varepsilon_z(x) = \varepsilon_{z,0} \left[ 1 + 6\alpha \frac{x}{d} \left( 1 - \frac{x}{d} \right) \right],$$



# Universal behavior of a dispersive Dirac cone

Double well profile

$$f_{\text{dw}}(x) = 1 - 3.2x + 13.2x^2 - 20x^3 + 10x^4$$





# Outline

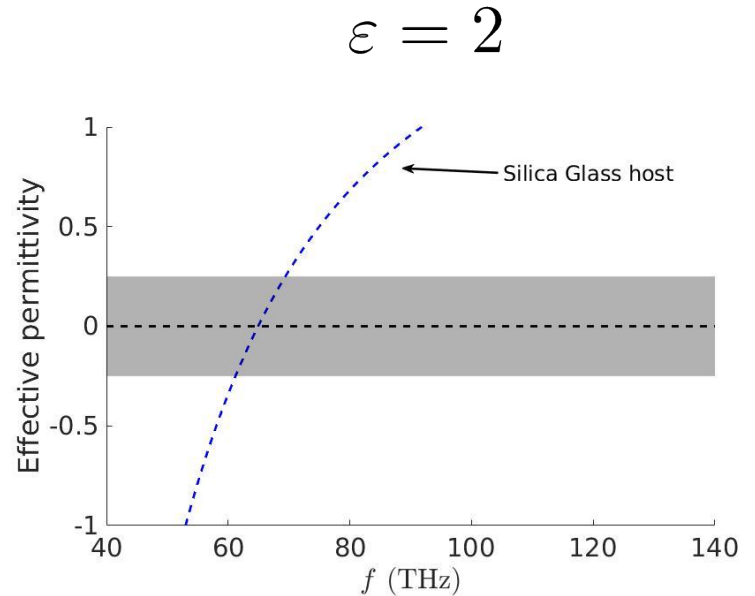
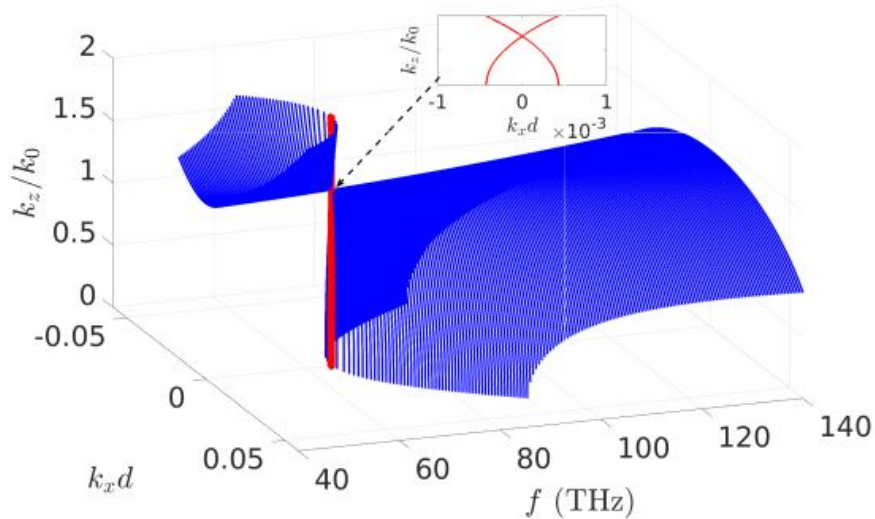
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# Expanding the ENZ frequency window

Very narrow frequency window with ENZ properties



# Lorentz dispersive host

Add a new Dirac point expanding ENZ frequency range

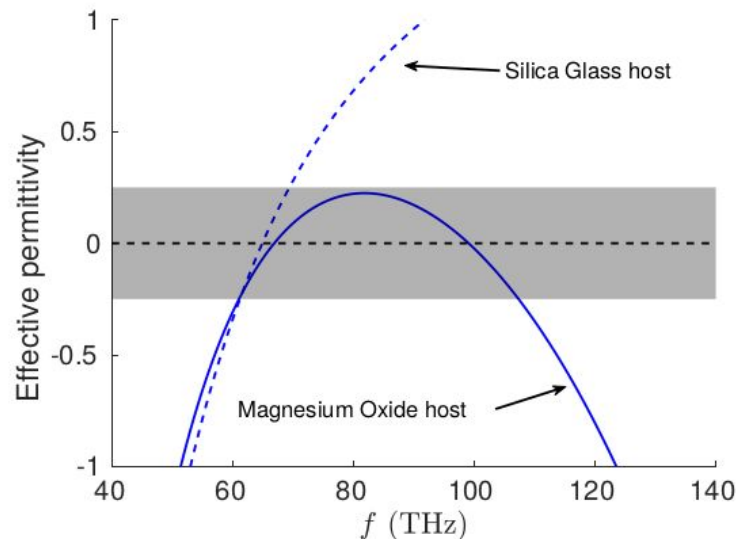
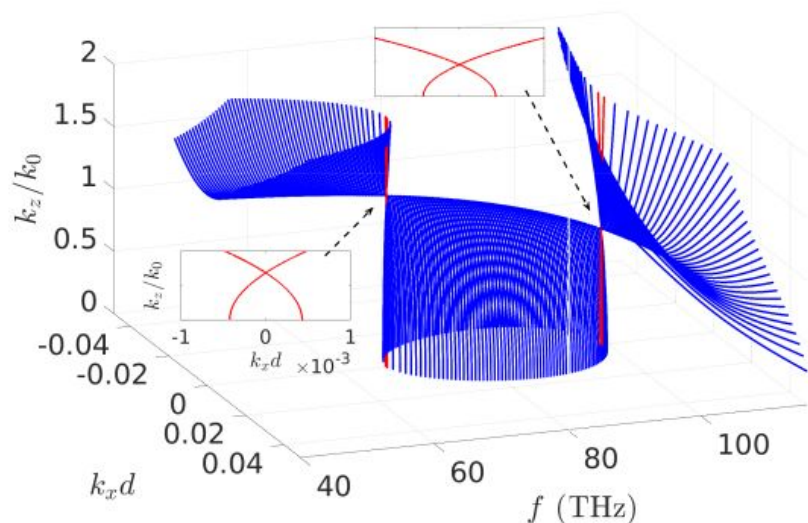
$$\varepsilon(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{\omega_0^2 - \omega^2 + i\omega\Gamma}$$

$$\varepsilon_\infty = 11.2$$

$$\varepsilon_s = 2.6$$

$$\Gamma = 0$$

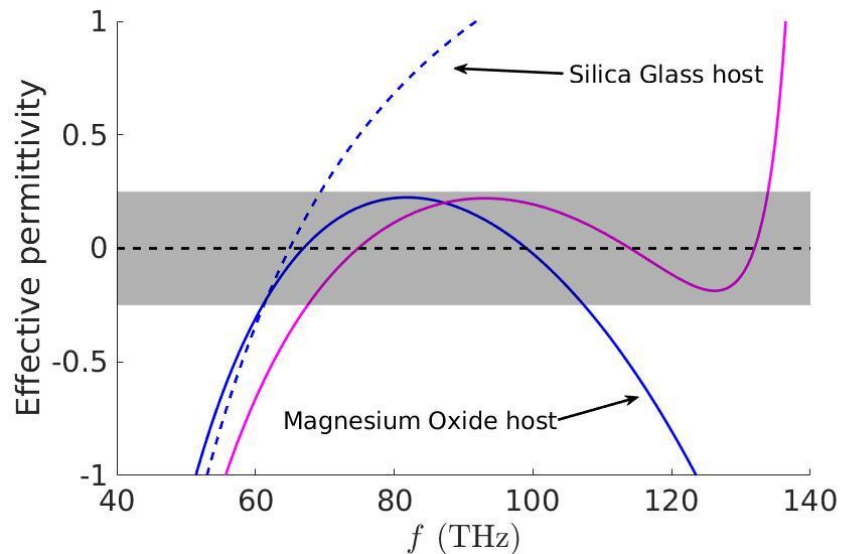
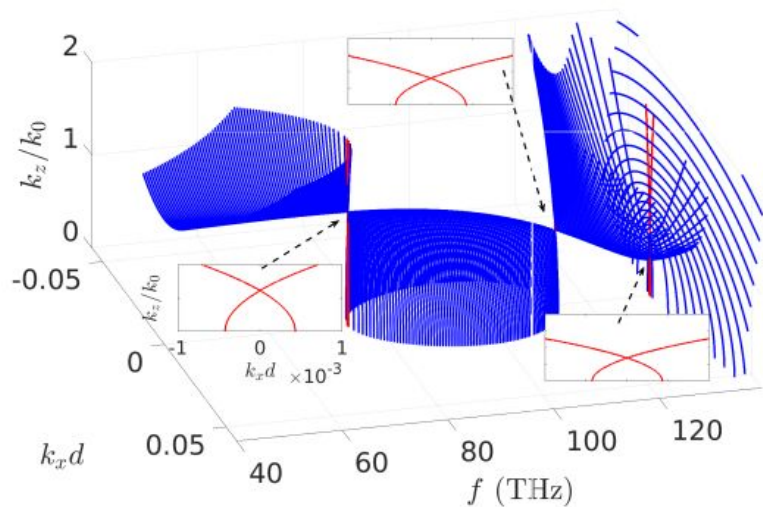
$$\omega_0 = 1\text{eV} (f = 242.8\text{THz})$$



# Multi-Oscillator Lorentz dispersive host

Add more Dirac points and expanding more the ENZ window

$$\epsilon(\omega) = \epsilon_{\infty} + \sum_i^N \frac{g_i \omega_{0i}^2}{\omega_{0i}^2 - \omega^2 + i\omega\Gamma_i},$$



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# General formula for the effective medium

A rigorous formulation for the effective dielectric function

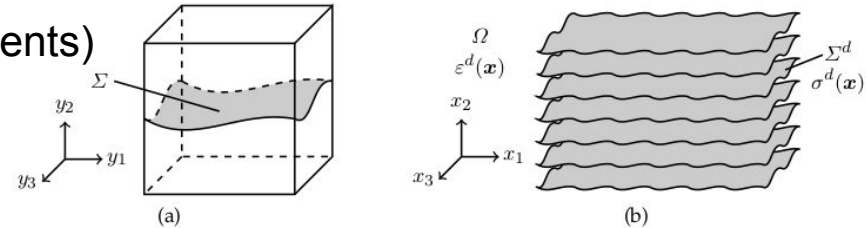
Arbitrary shape of a 2D material as the building element

Periodic structure in one, two, or three dimensions

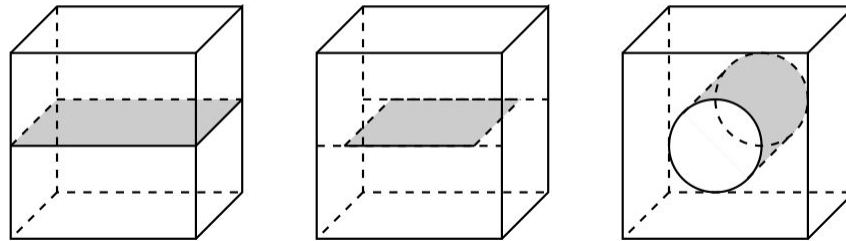
Finite and edge state effects (surface + line currents)

Finite number of structural periods

Spatial & frequency-dependent host permittivity



Choose your 2D element:  
planar, ribbon, tube



# Conclusion

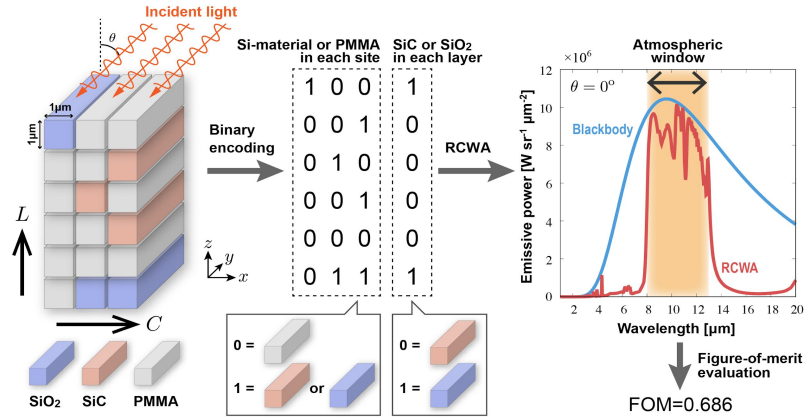
- A systematic way to design crystals with ENZ behavior
  - Tuning dynamically the optical properties
  - Dirac dispersion indicates ENZ behavior
- Universality of Dirac dispersion and ENZ for 2D plasmonic crystals with spatial-dependent host
- Expand the ENZ frequency window with Lorentz dispersive host
- A rigorous formulation for a general case of plasmonic crystal structure:  
A general ENZ condition

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[https://scholar.harvard.edu/marios\\_matthaiakis](https://scholar.harvard.edu/marios_matthaiakis)

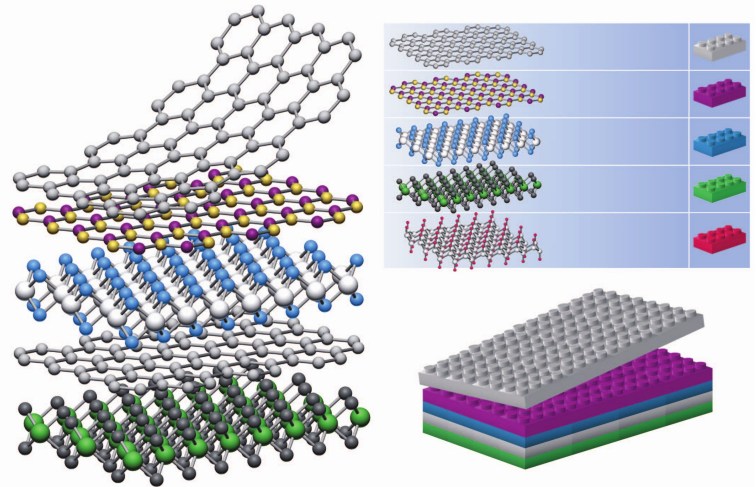
# A promising direction in engineering

## Machine Learning for designing new metamaterials



Kitai et al. Arxiv 1902.06573

## Flatland multilayer heterostructures



### Scheme:

Set target properties

Define a periodic structure

Choose the building elements

Let ML to design the optimal configuration

Geim et al. Nature **499** 2019



# Acknowledgments



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**INSTITUTE FOR APPLIED  
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Co-authors:

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Wei Xi Boo  
Efthimios Kaxiras

**ODYSSEY**  
HARVARD FAS  
RESEARCH COMPUTING

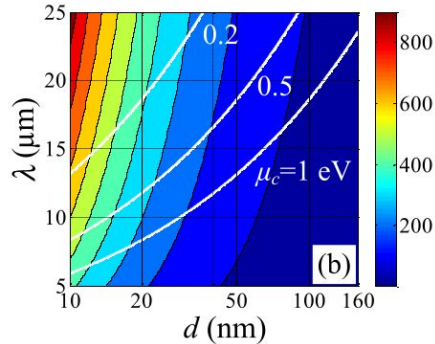
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# Supplementary Material

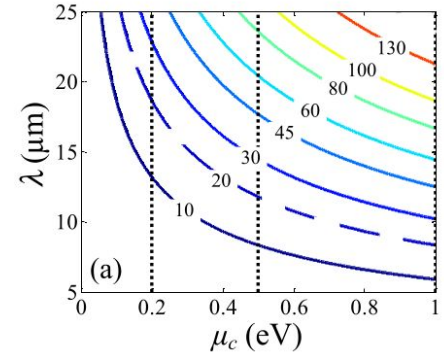
# General Investigation (maps)

- Combinations of  $\mu_c$  and  $\lambda$  leading to PDP & ENZ ( $\xi$  is plotted in nm).
- ✓ A structure with arbitrary  $d$  can be fabricated and then with suitable choice of  $\mu_c$  and  $\lambda$  we achieve ENZ behavior.

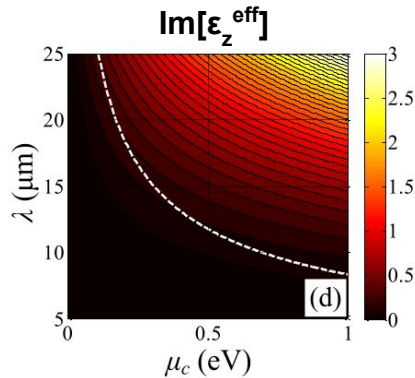
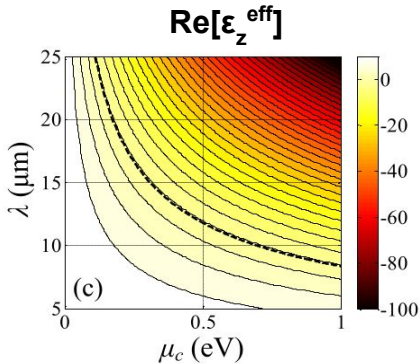


$$\frac{L}{d} = \sqrt{\frac{2}{\epsilon_z}} \sqrt{\frac{\text{Im}[\sigma_s]}{\text{Re}[\sigma_s]}} \frac{1}{k_0 d}$$

For Drude:  
 $L \sim \lambda^{1/2}$



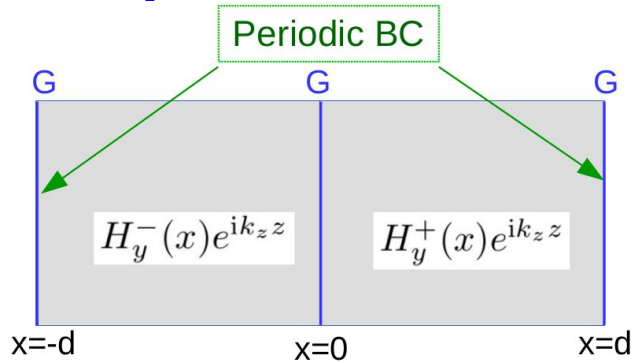
The propagation distance  $L/d$  of a plasmonic mode for all  $\lambda$ ,  $d$  and  $\mu_c$  combinations leading to ENZ.



Effective permittivity for  $\lambda$  &  $\mu_c$  combinations and fixed period  $d=20\text{nm}$ .

- Dashed lines indicate the ENZ regime.
- ✓ Low losses in the ENZ region.
- ✓ Very negative  $\epsilon$  achieved but accompanied with high losses.

# Dispersion Relation



- Assuming that Graphene carries surface current  $J = \sigma E_z$ .
- Periodicity: The eigenmodes are Bloch waves and arranged in bands.

$$H_y^+(x) = H_y^-(x - d)e^{ik_x d}$$

$$F(k_x, k_z) = \cos(k_x d) - \left[ \cosh(\kappa d) - \frac{\xi \kappa}{2} \sinh(\kappa d) \right] = 0$$

- ▶ Assume very dense grid:  $\kappa d \ll 1$
- ▶ Around Brillouin center:  $k_x \sim 0$ .

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

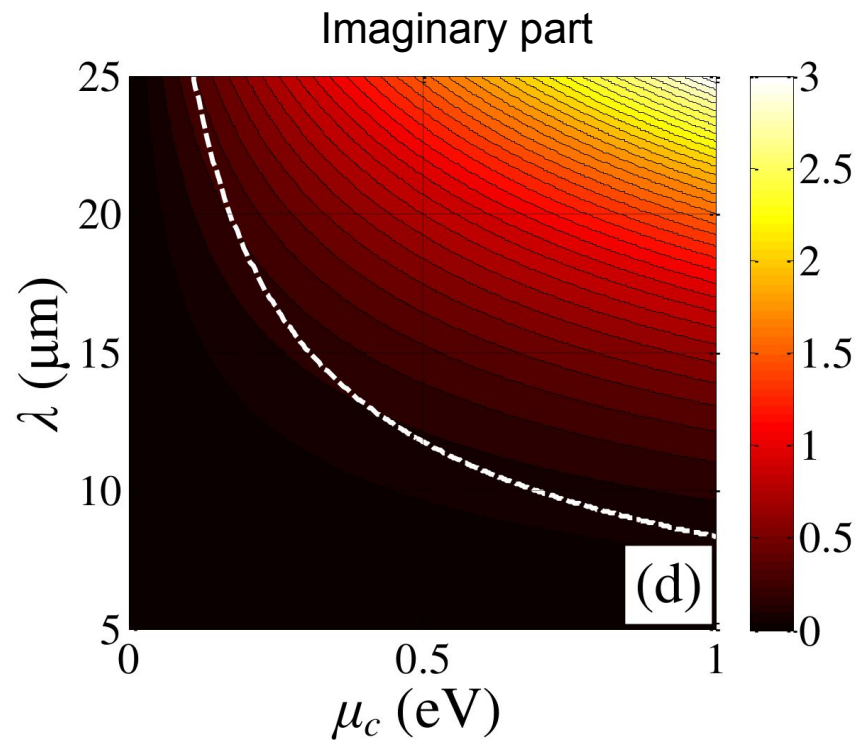
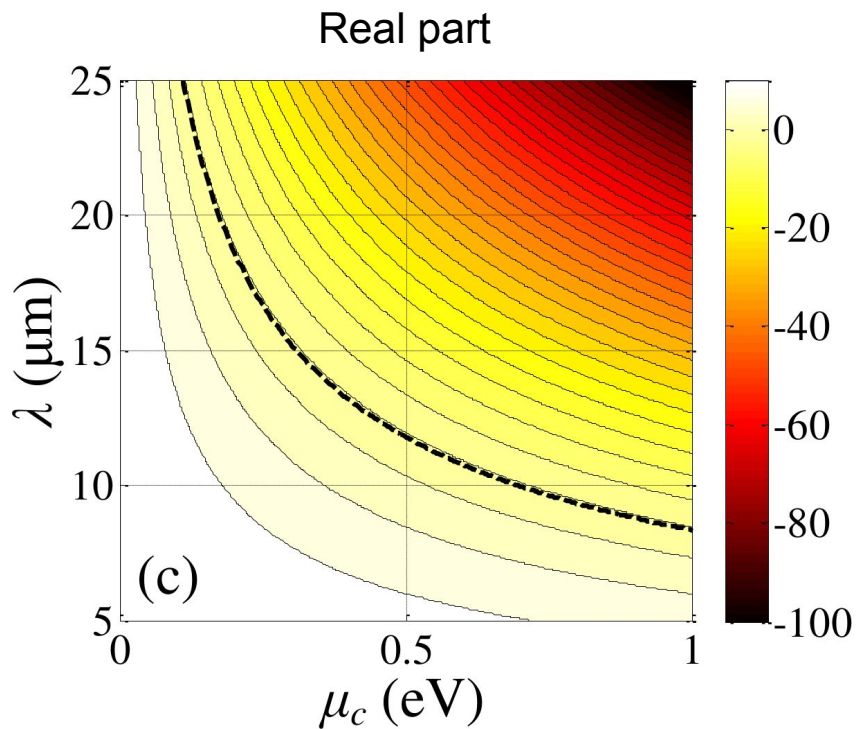
$$\kappa = \sqrt{\frac{\epsilon_z}{\epsilon_x} (k_z^2 - k_0^2 \epsilon_x)}.$$

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

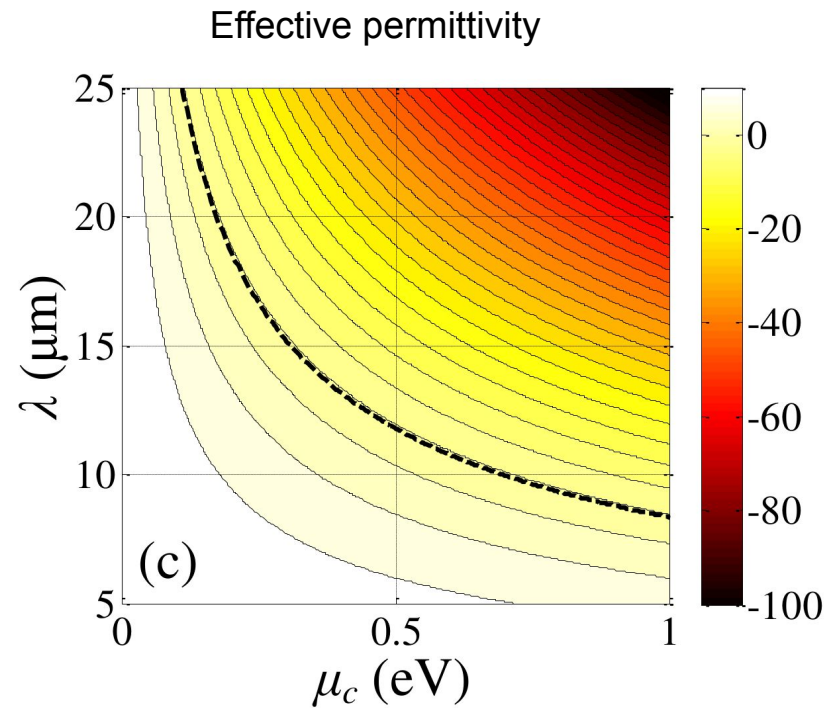
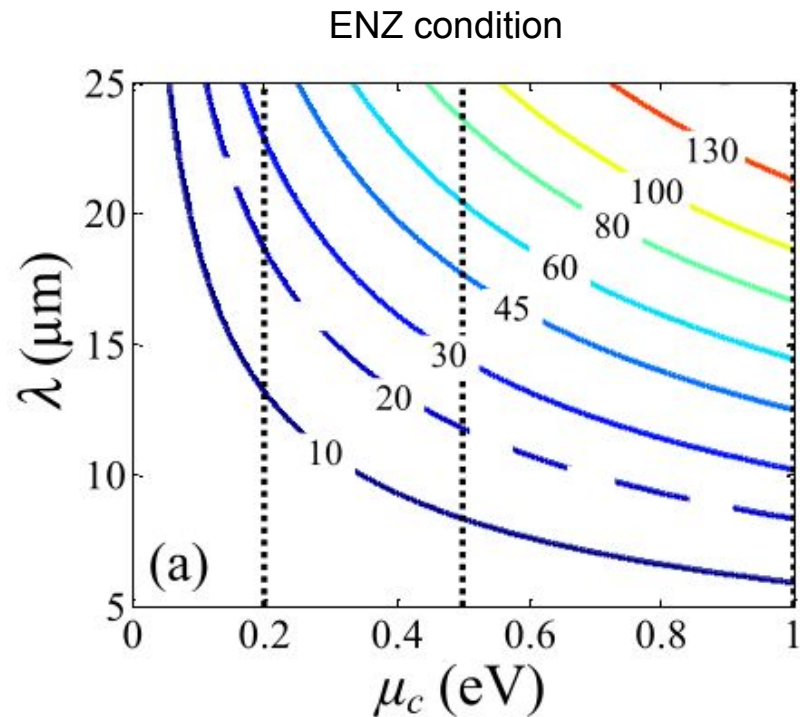
- $d > \xi$ : Weak Plasmon Coupling → Elliptic Band
- $d = \xi$ : Critical Plasmon Coupling → Two Linear Bands
- $d < \xi$ : Strong Plasmon Coupling → Hyperbolic Band

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

# Effective dielectric function



# Tunable EM properties



# Universal behavior of a dispersive Dirac cone

Dirac dispersion and ENZ is a universal property of plasmonic crystals consisting of 2d metals in host with space-dependent permittivity

General dispersion relation:

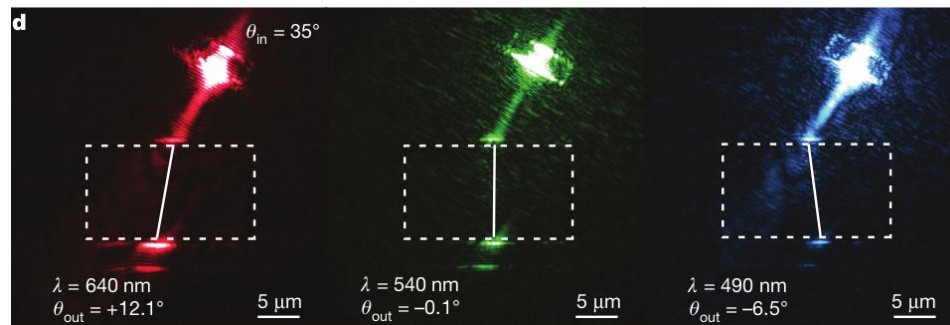
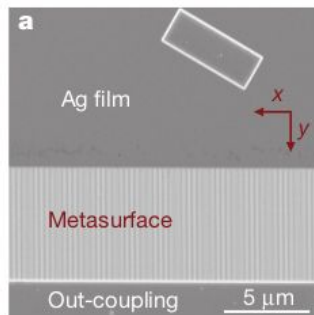
$$D[\mathbf{k}] = \det \left( \begin{array}{cc} \mathcal{E}_{(1)}(d) & \mathcal{E}_{(2)}(d) \\ \mathcal{E}'_{(1)}(d) & \mathcal{E}'_{(2)}(d) \end{array} \right) - e^{ik_x d} \begin{bmatrix} 1 & 0 \\ -i(\sigma/\omega)\kappa(k_z) & 1 \end{bmatrix} = 0.$$

Universal condition for ENZ

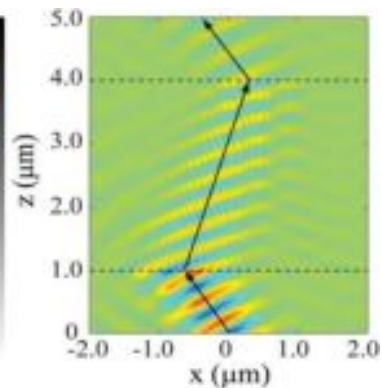
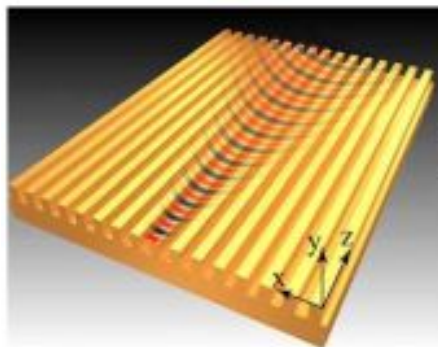
$$d_0 = \xi_0 \left[ \int_0^1 f(x) dx \right]^{-1}, \quad \frac{\varepsilon_z^{\text{eff}}}{\varepsilon_{z,0}} = \xi_0 \left( \frac{1}{d_0} - \frac{1}{d} \right).$$



# Multilayer Metamaterial



Hyperbolic metasurface.  
Nat. Lett. **522** 2015



Negative refraction. APL 2013

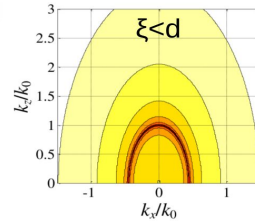
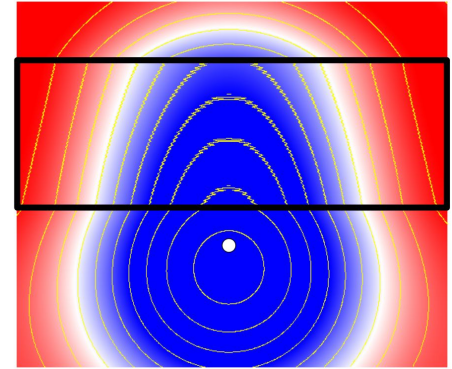


# Numerical EM wave simulations (vids)

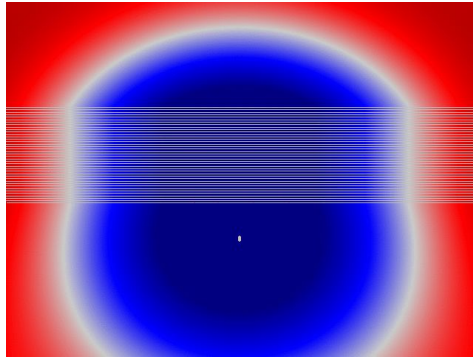
- 40 graphene layers embedded in MoS<sub>2</sub> host ( $\epsilon_x=3.5$ ,  $\epsilon_z=13$ ,  $d=20.8$  nm).
- Drude model for graphene conductivity.
- $\lambda_0=12$   $\mu\text{m}$  (THz regime).
- 2D magnetic dipole source.

COMSOL  
simulations

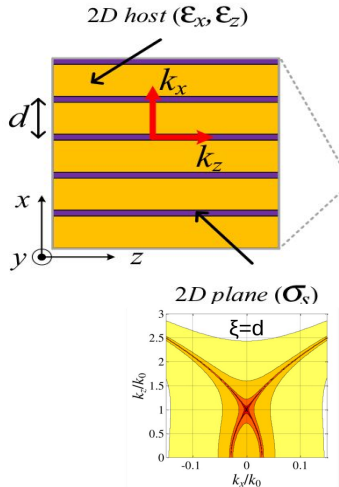
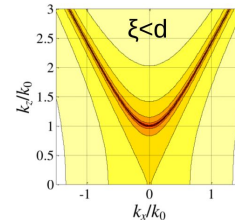
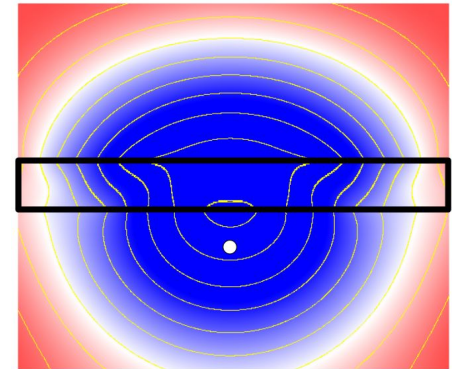
Weak plasmon coupling



Plasmonic Dirac Point



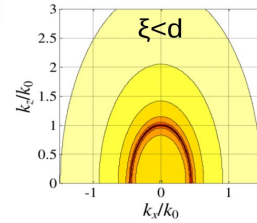
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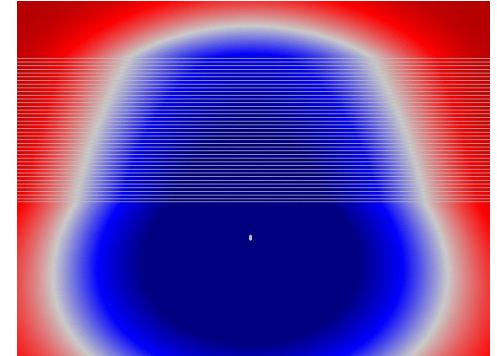
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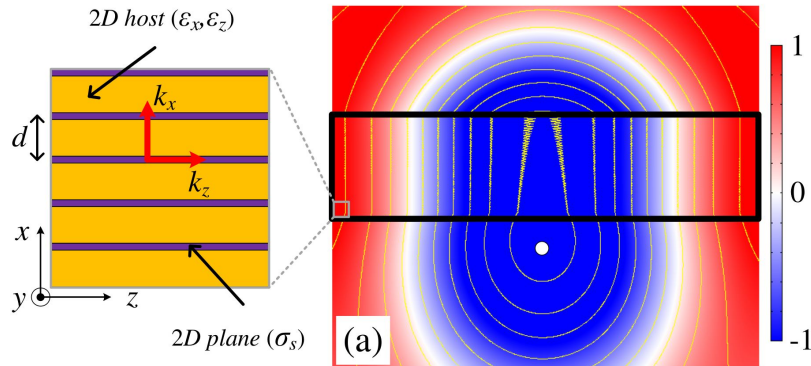
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simulations



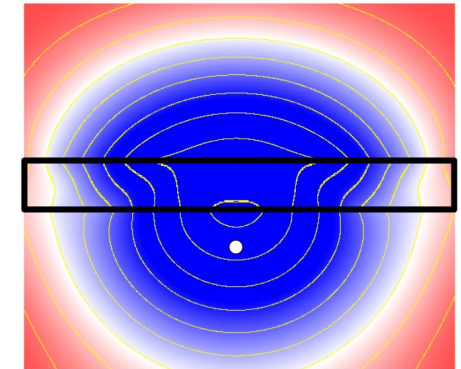
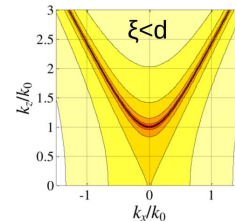
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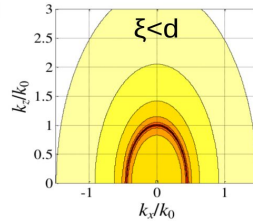
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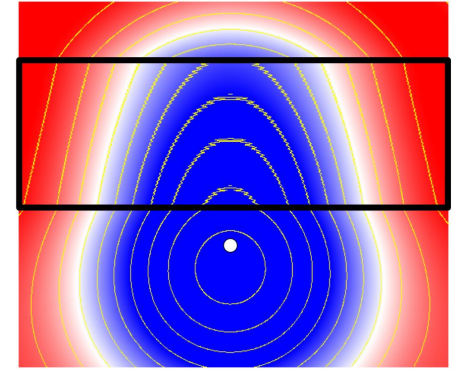
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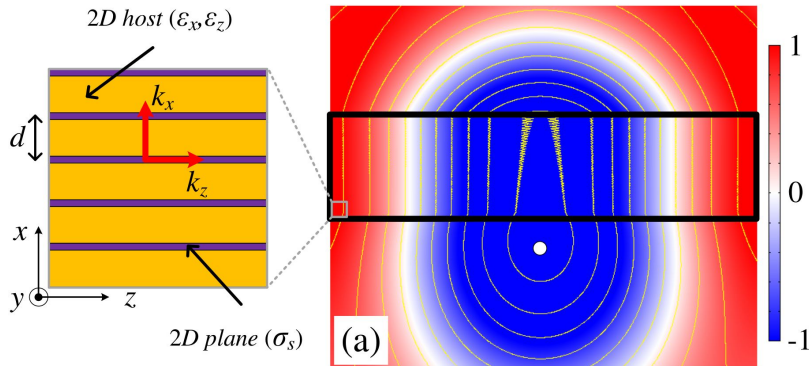
COMSOL  
simulations



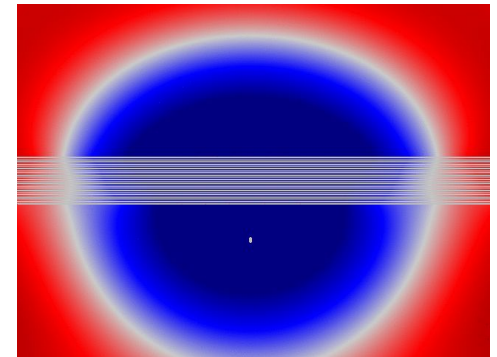
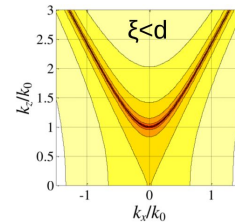
Weak plasmon coupling



Plasmonic Dirac Point



Strong plasmon coupling



# ENZ properties

Wave propagation with no dispersion and with no phase delay

Propagation through narrow channels

Bending over arbitrary angles

Ultra fast phase transitions

Hiding objects (cloaking)

