# Bottom-up Synthesis of Nanographenes and its Effects on Electrical and Optical Properties

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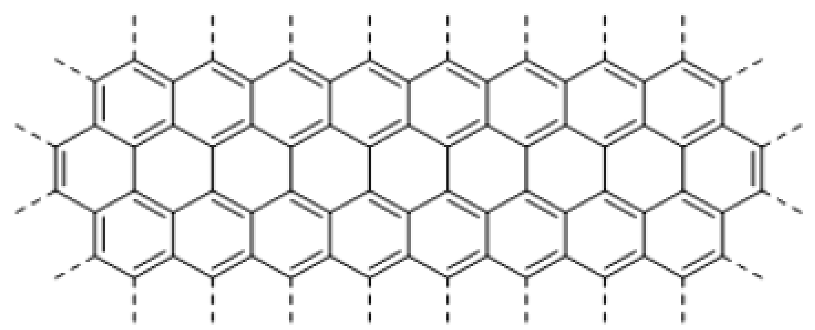
## Graphenes and Nanographenes

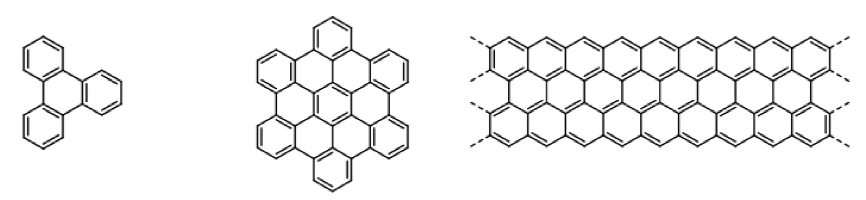
Graphene



Nanographene

Polycyclic Aromatic Hydrocarbons (PAH)s

Graphene Nanoribbons (GNR)s



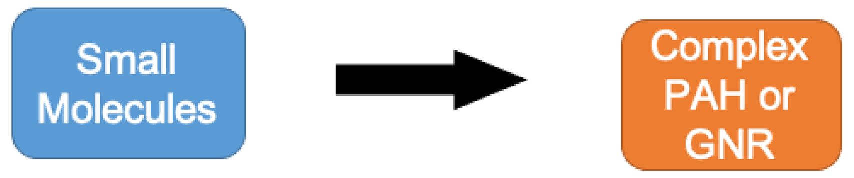
Increasing size and complexity

- Infinite 2D sheet of connected $sp^2$ carbons
- Zero band gap
- Excellent conductivity

Tunable HOMO→LUMO gap depending upon:

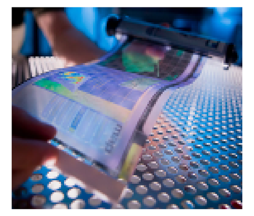
- size
- 3D Shape (planar vs. curved)
- heteroatom doping

"Bottom-Up" Synthesis of Nanographenes

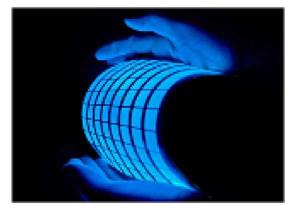



Solution synthesis allows control over key parameters such as heteroatom doping, edge structure, and size!

Nanographenes as Organic Semiconductors

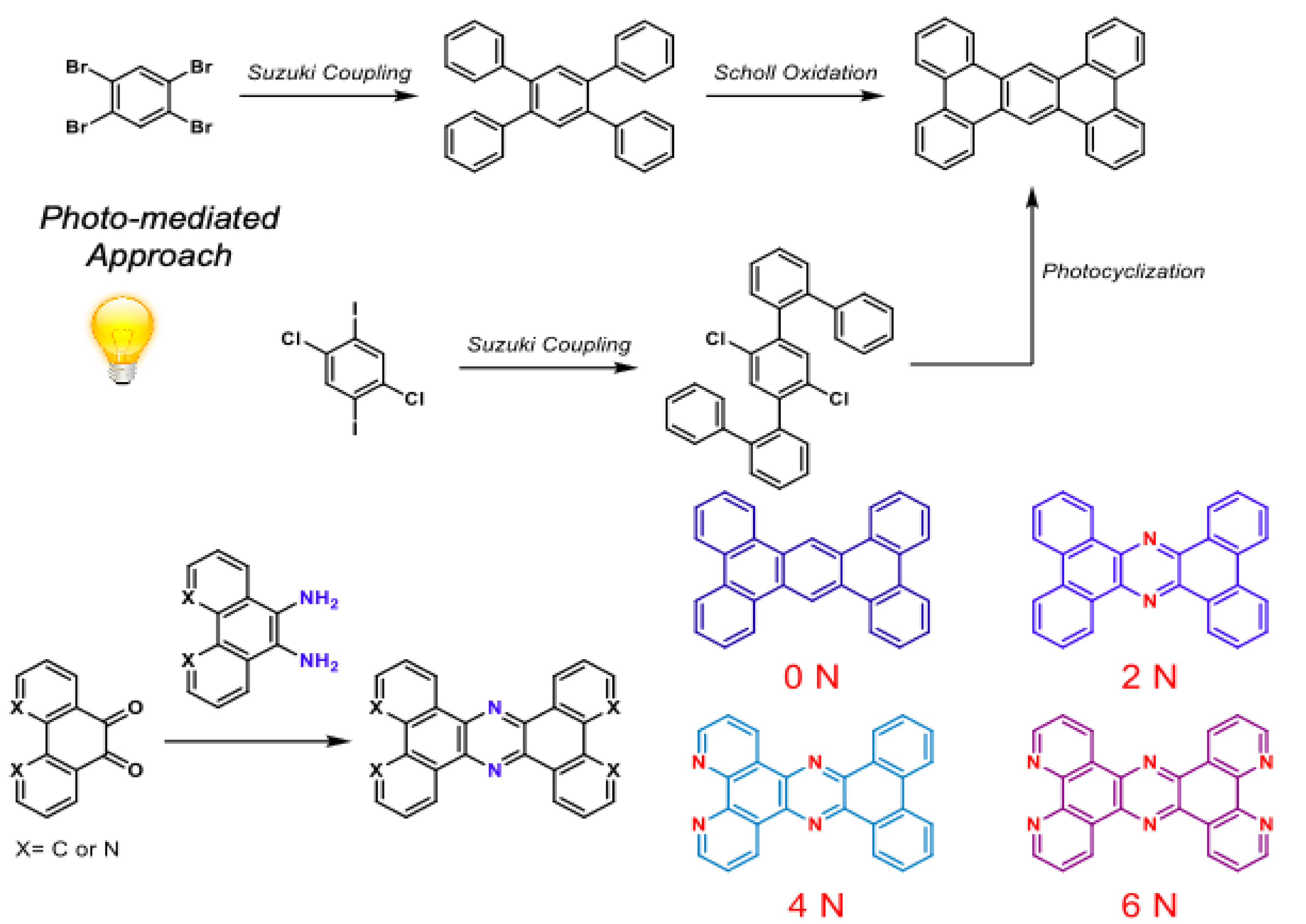


Organic Field Effect Transistors (OFET)

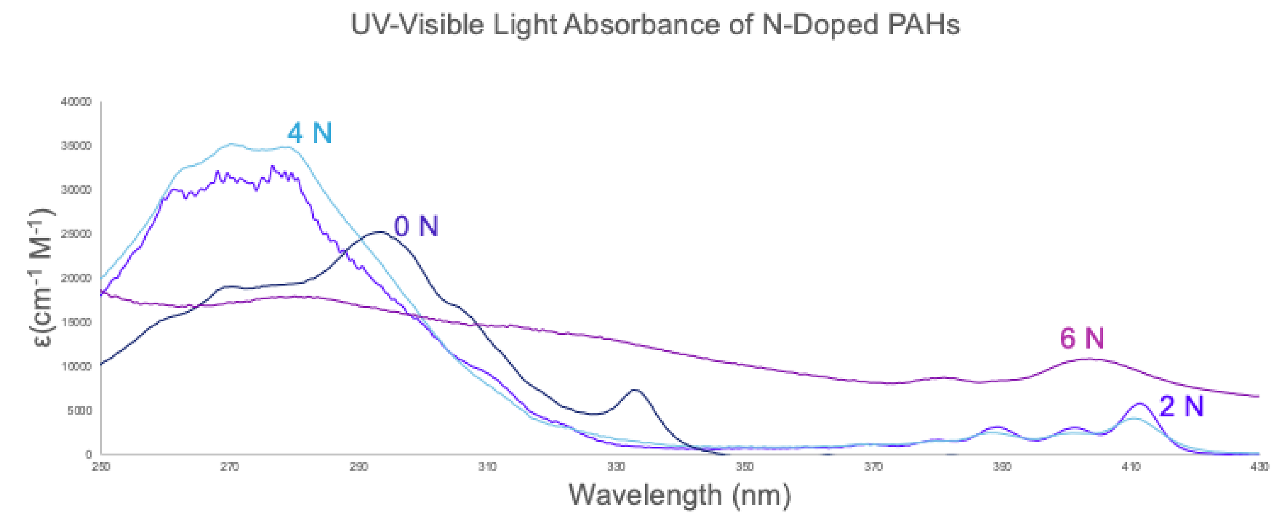


Organic Light-Emitting Diodes (OLED)

## Synthesis of Nanographene Series



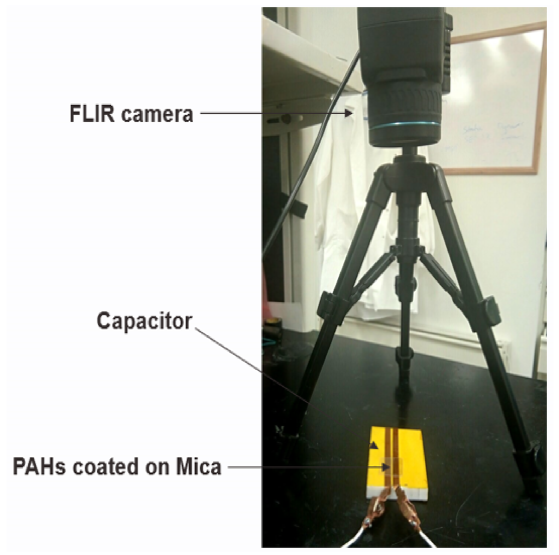

## Optical Properties of Nanographene Series (UV Spectra)



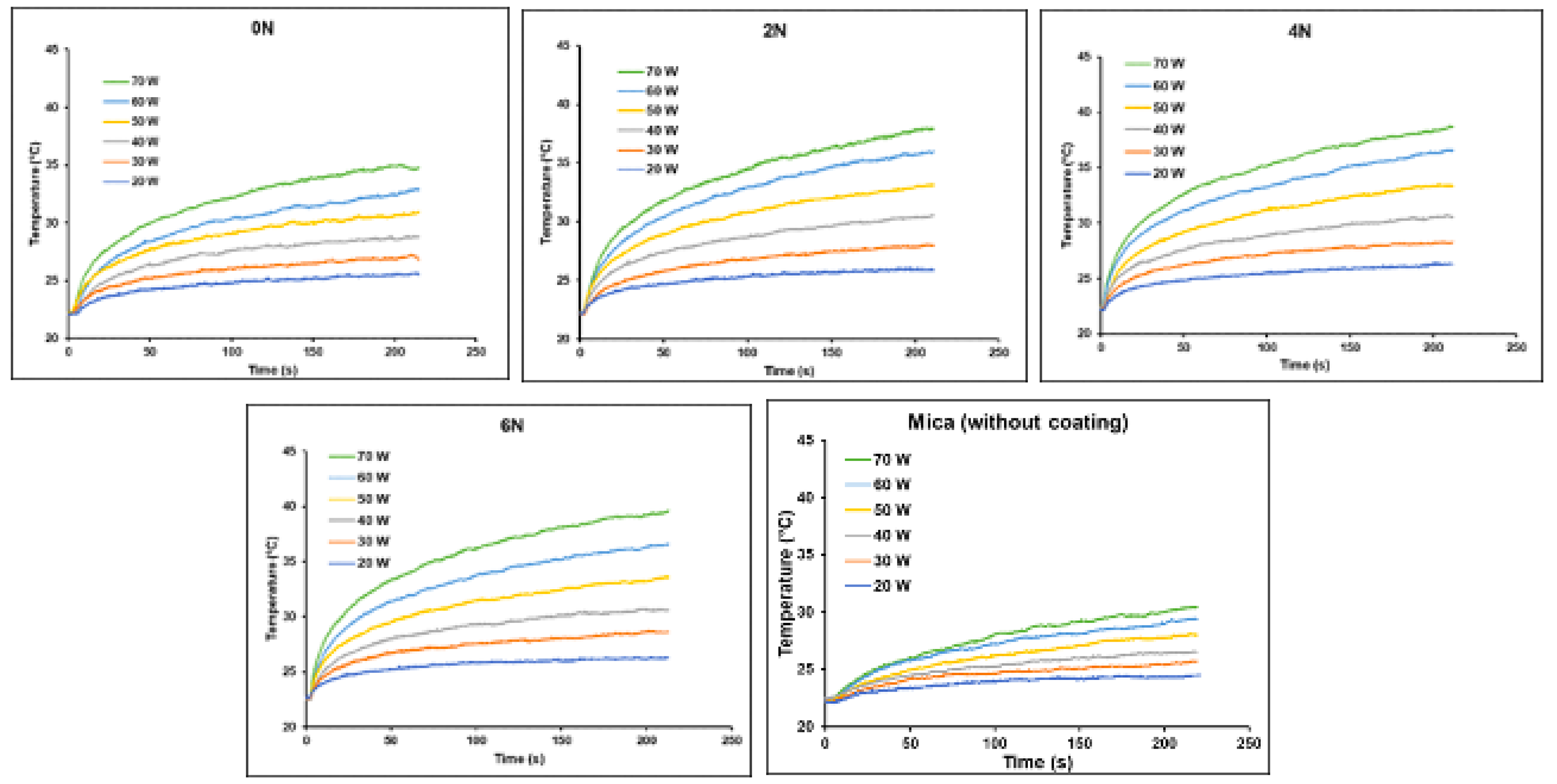

## Comparison of Radio Frequency (RF) response of PAHs

Preliminary Experiment:

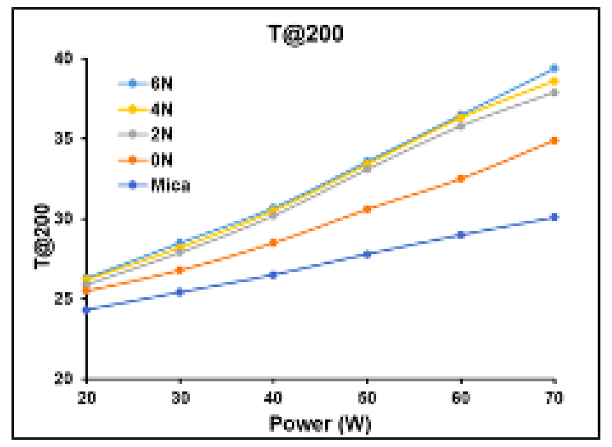
1. 1 mg of each of the three samples were spin-coated at 1000 rpm for 1 min on 5 Mica (substrate) pieces (Dimension: 2.5 cm × 2.5 cm).
2. RF setup consists of a fringing field capacitor which has two copper electrodes that are connected to an amplifier which in turn, supplied the RF power. PAHs coated on Mica sheets were placed on this capacitor before RF power is supplied.
3. An optimum frequency of 104 MHz and different powers were supplied to them to check the RF response. [Note that Mica does not strongly affect the field.]




Maximum Temperature-Time profile



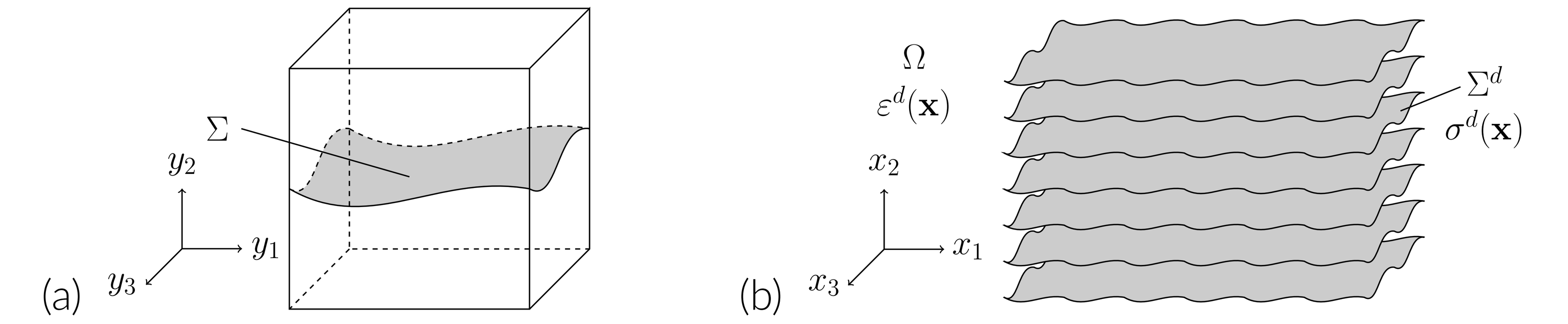

Temperature @ 200 C for PAHs at different powers




***Observation**: RF thermal response of PAHs increases with increase in N content*

## Theoretical Problem Setup

We carry out the homogenization of time-harmonic Maxwell's equations and in a periodic layered structure of 2D metallic sheets immersed in a heterogeneous and anisotropic dielectric medium. The following figure shows the geometric orientation of the layered structure.




**Schematic of geometry:** (a) The unit cell, $Y = [0,1]^3$, with microstructure $\Sigma$, a conducting sheet. (b) Computational domain $\Omega$ with rescaled periodic layers $\Sigma^d$ and spatially dependent surface conductivity $\sigma^d(\mathbf{x})$. The ambient medium has a heterogeneous permittivity, $\varepsilon^d(\mathbf{x})$.

## Homogenized Macroscale Problem and Variational formulation

Consider an electromagnetic wave $(\mathbf{E}^d, \mathbf{H}^d)$ in a surface $\Omega\backslash\Sigma^d$. The Maxwell's equations for this wave are,

$$\begin{cases} \nabla \times \mathbf{E}^d = i\omega\mu\mathbf{H}^d, \\ \nabla \times \mathbf{H}^d = i\omega\varepsilon^d\mathbf{E}^d + \mathbf{J}^d, \end{cases} \quad \text{in } \Omega$$

where $\mathbf{J}^d = (\sigma^d\mathbf{E}^d_T)\delta_{\Sigma^d} + \mathbf{J}_a$. The boundary condition is $\frac{1}{\mu}(\nabla \times \mathbf{E}^d) \times \nu = i\omega\lambda\mathbf{E}^d_t$ on $\partial\Omega$. Using a smooth testing function $\psi$ and plugging in the boundary conditions, we formulate the variational form,

$$\int_\Omega \frac{1}{\mu}(\nabla\times\mathbf{E}^d)\cdot(\nabla\times\bar{\psi})dx - \int_{\partial\Omega} i\omega\lambda\mathbf{E}^d\cdot\bar{\psi}_T do_x - \int_\Omega \omega^2\varepsilon^d\mathbf{E}^d\cdot\bar{\psi}dx - \int_{\Sigma^d} i\omega\sigma^d\mathbf{E}^d_T\cdot\bar{\psi}_T do_x = \int_\Omega i\omega\mathbf{J}_a\cdot\bar{\psi}dx.$$

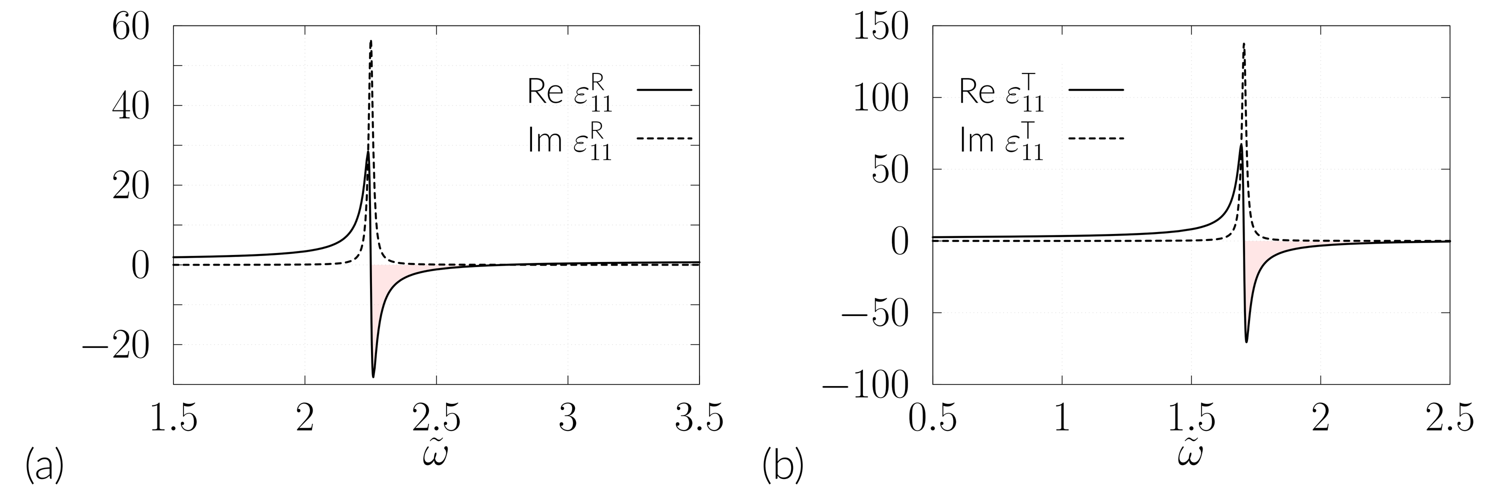
We define an effective tensor:

$$\varepsilon^{\text{eff}}_{ij}(x,\omega,\Sigma,\sigma) = \int_Y \varepsilon(x,y)(e_j + \nabla\chi_j(x,y))\cdot(e_i + \nabla\overline{\chi}_i(x,y))\,\mathrm{d}y - \frac{1}{i\omega}\int_\Sigma \sigma(x,y)(e_j + \nabla\chi_j(x,y))\cdot(e_i + \nabla\overline{\chi}_i(x,y))\,\mathrm{d}o_y.$$

and the cell problem $\chi_i \in H^1_{\text{per}}(Y)$, $i = 1,2,3$

$$\int_Y \varepsilon(x,y)(e_i + \nabla\chi_i(x,y))\cdot\nabla\psi(y)\,\mathrm{d}y - \frac{1}{i\omega}\int_\Sigma \sigma(x,y)(e_i + \nabla\chi_i(x,y))\cdot\nabla\psi(y)\,\mathrm{d}o_y = 0$$

## Optical Response of Plasmonic Nanographenes




Plots of real and imaginary parts of matrix elements of $\varepsilon^{\text{eff}}$ as a function of frequency. (a) $\varepsilon^R_{11}$ for nanoribbons; and (b) $\varepsilon^T_{11}$ or $\varepsilon^T_{22}$ ($\varepsilon^T_{11} = \varepsilon^T_{22}$) for nanotubes. The shaded area indicates the frequency regime for negative real part in each case.

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