Frontiers in device engineering:

Synthesis for non-intuitive design

High-productivity design tools for 21st century nano-technology

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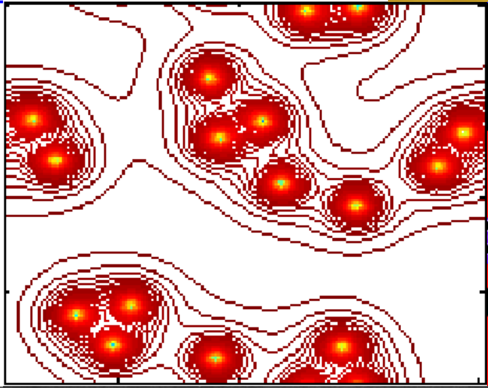
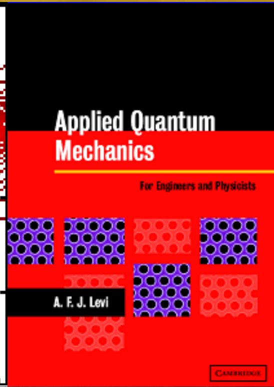
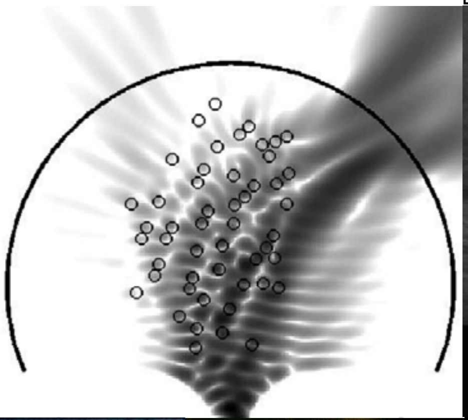
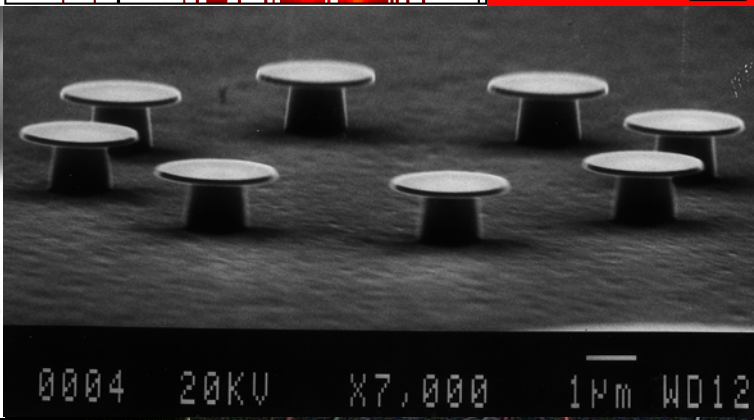
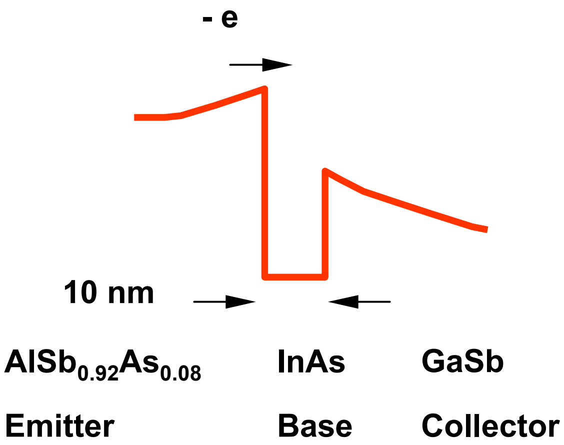
- **Adaptive quantum design of small systems**
  - Device synthesis
    - Atoms-up configurations for function
  - Optimization
    - Non-intuitive design and discovery
- **Nanophotonics**
  - Scaled semiconductor lasers
    - Sub-wavelength cavity design, switching
  - Electromagnetic scattering
    - Aperiodic dielectric structures
- **Semiconductor device physics**
  - Nonequilibrium electron transport
    - HBTs, NETs
- **System engineering**
  - High performance electronics
    - Interconnects
    - RF systems

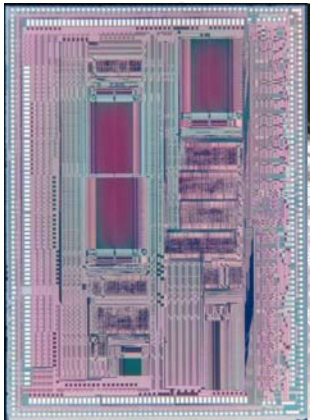


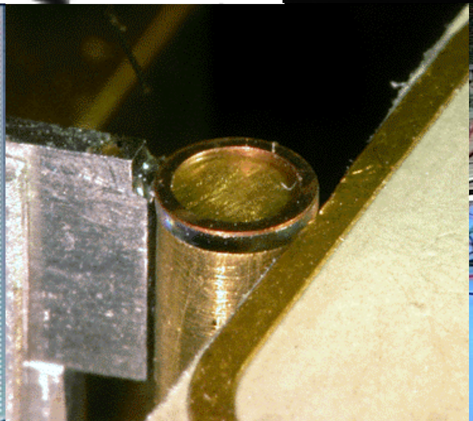


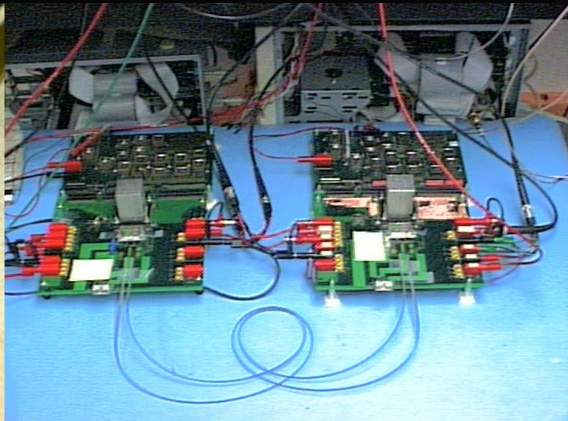






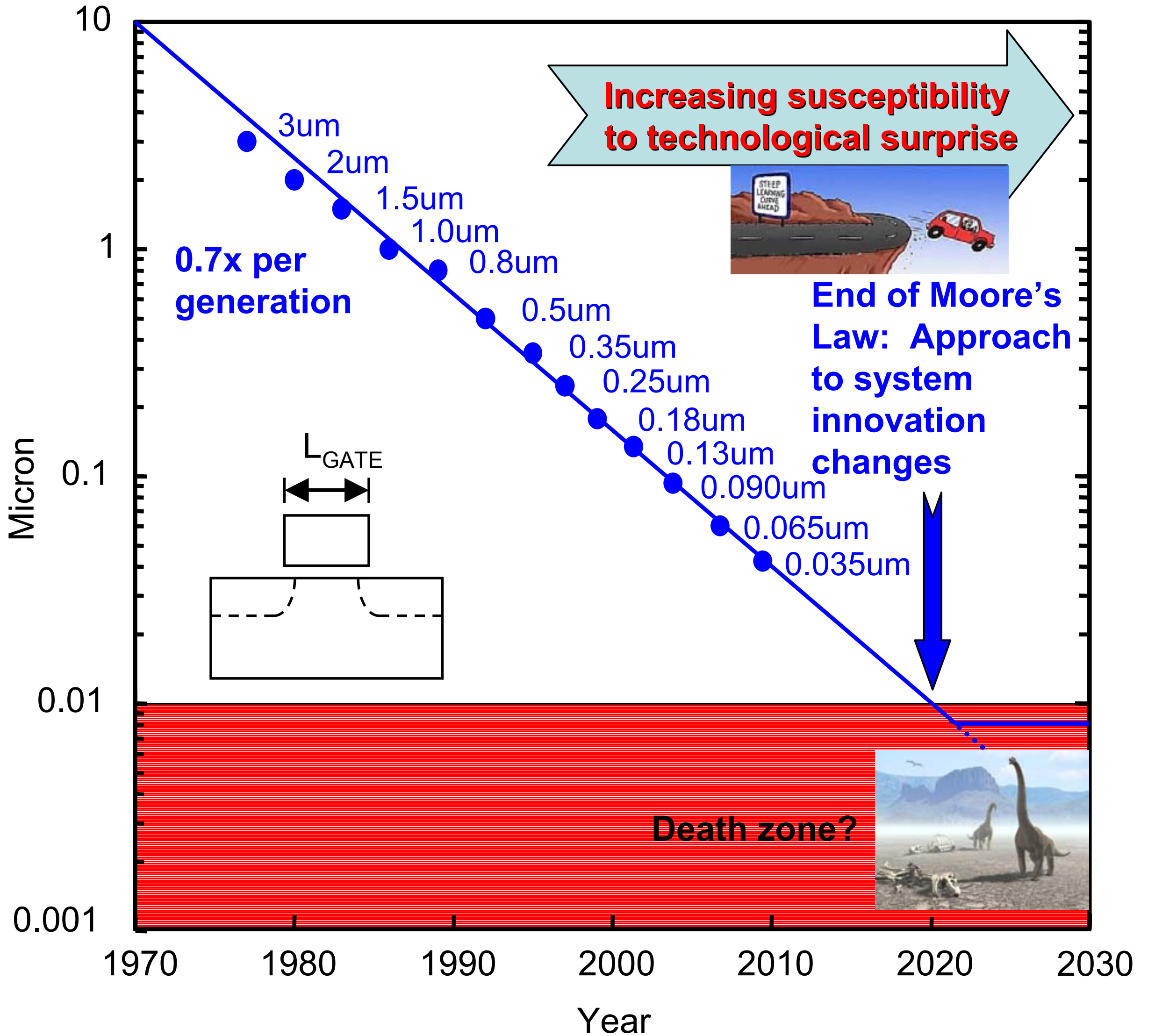






Technology mega-trends: Transistor scaling will flat-line

- Preparing for the end of Moore's Law
- After 2020:
  - Rules for building systems changes
  - Increased risk of technological surprise
- ***Solution*:** Create design tools that contain the knowledge to secure systems beyond 2020 endpoint
  - **Increase efficiency of scientific discovery and technological development**



What is the scaling paradigm in technology beyond 2020?

- ***Not*** **physical scaling of device size to increase number of devices per mm^2 and thereby increase system functionality**
- **It is *increased functionality via* manipulation of *new degrees of freedom***
  - **Single electron states in a nano particle**
    - **Single electron picture**
  - **Interacting electrons in presence of coulomb interaction**
    - **Collective excitations (e.g. plasmonics)**
  - **Hybridization**
    - **Bonding and chemical specificity**
  - **Electron spin**
    - **Magnetization**
  - **Light-matter interaction**
    - **Strong coupling**
  - **Nonequilibrium processes**
    - **fs time scales**
- ***Efficient* exploitation requires new design tools**
  - **Many degrees of freedom**
  - **Initially non-intuitive configurations**

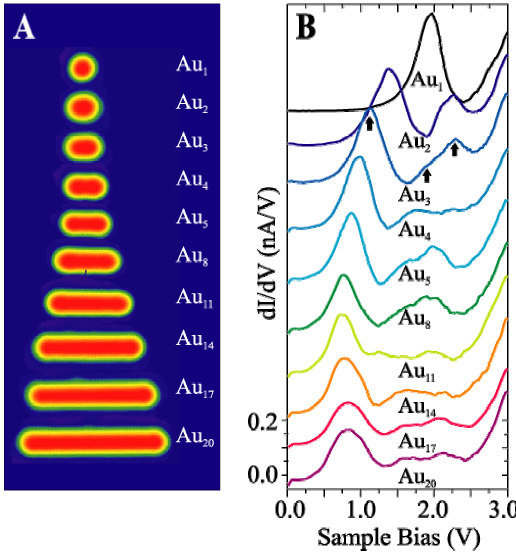
Example: Atoms-up device synthesis for quantum systems: Broken symmetry enables function

- ***N*** **particle system of atoms with overlap of atomic wave functions dependent on distance,** $t_{\mathbf{r},\mathbf{r}'} = |\mathbf{r}-\mathbf{r}'|^{-\alpha}$ **e.g.** α **= 3**
- **Hamiltonian includes interactions between *all* atoms**

$$\hat{H} = -\sum_{\langle \mathbf{r},\mathbf{r}' \rangle} t_{\mathbf{r},\mathbf{r}'} \left(\hat{c}_{\mathbf{r}}^{\dagger} \hat{c}_{\mathbf{r}'} + \hat{c}_{\mathbf{r}} \hat{c}_{\mathbf{r}'}^{\dagger} \right)$$

- **Numerically determine eigenvalues and eigenstates of system with Hamiltonian**

$$\hat{H} = \begin{bmatrix} 0 & t_{12} & t_{13} & . \\ t_{21} & 0 & t_{23} & . \\ t_{31} & t_{32} & 0 & . \\ . & . & . & . \end{bmatrix}$$



Example: Tailoring Electronic Properties of Atomic Chains Assembled by STM, N. Nilius and T. M. Wallis and W. Ho, Appl. Phys. A 80, 951-956 (2005)

- **Determine physical quantity of interest e.g. density of states** $N(E)$
  - **By *breaking translational symmetry* of the system the desired response can be obtained**
- **Compare with objective function and perform guided random walk to minimize** $\Delta = |N(E) - N_{\text{obj}}(E)| \to 0$

Example: Atoms-up system design using an optimizer

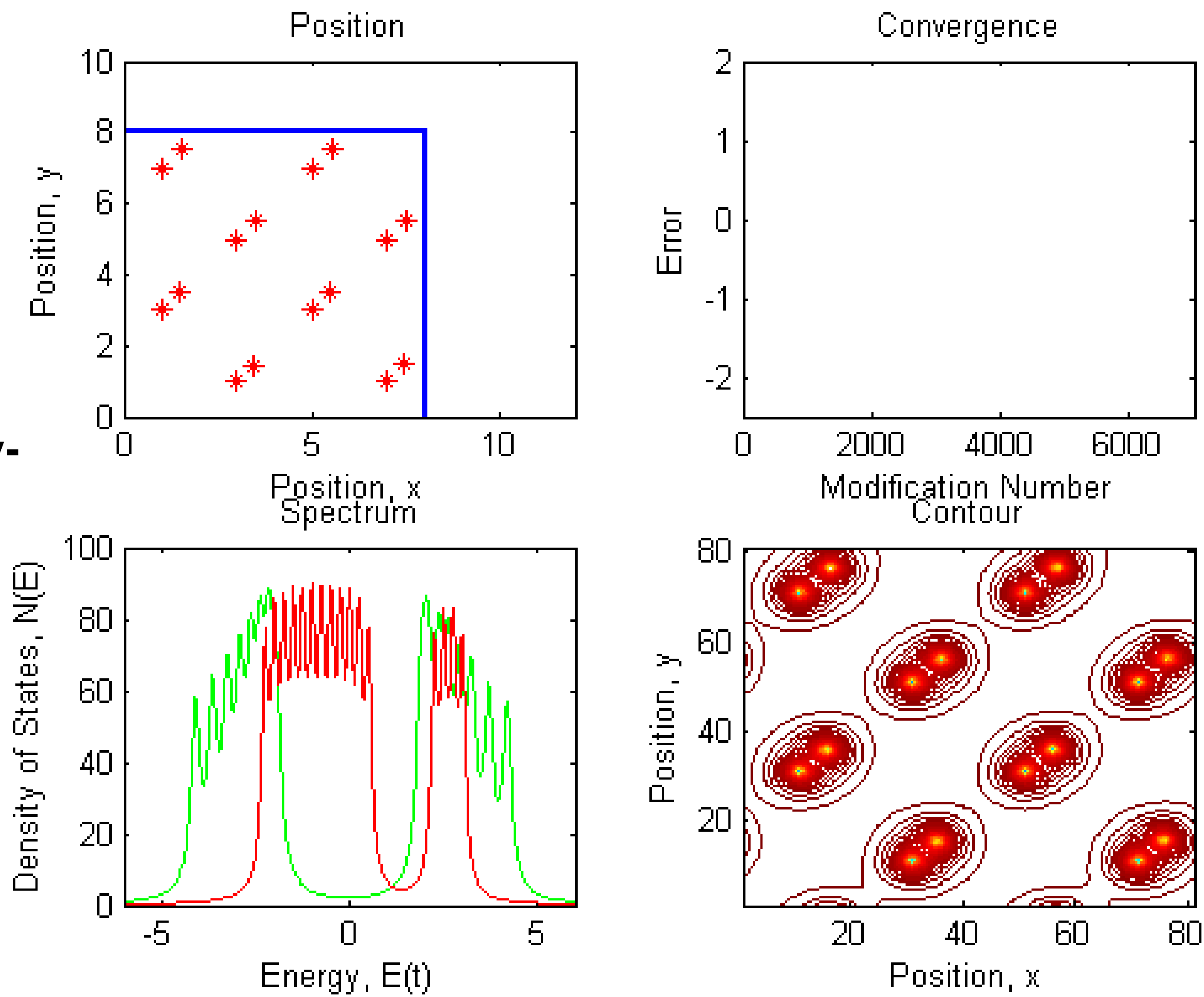
Visualization of adaptive algorithm:

- **Initial 2D periodic array of atoms**
- **Tight binding description of electrons**
- **Periodic boundary condition (blue line)**
- **Asymmetric density-of-states objective**

Break symmetry **to achieve objective density of states**

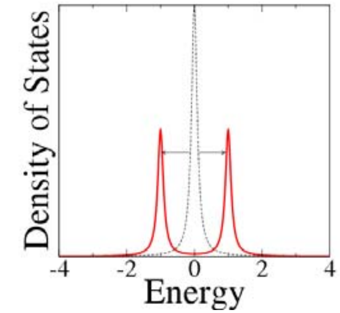
  - **Local update, guided random walk**

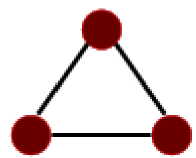
- ***Non-intuitive solution***
  - **New understanding**

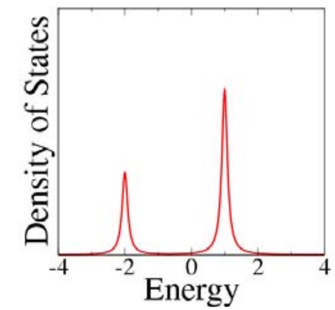


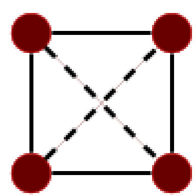
Learning from output of synthesis tools: Molecular building blocks in the dilute limit

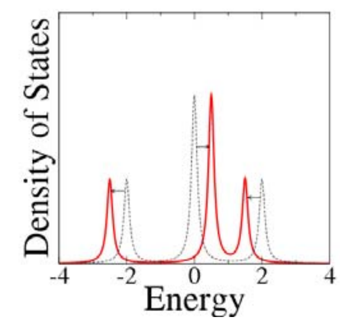
- Dimers:  $E = \pm t$



- Trimers:  $E = -2t, t, t$

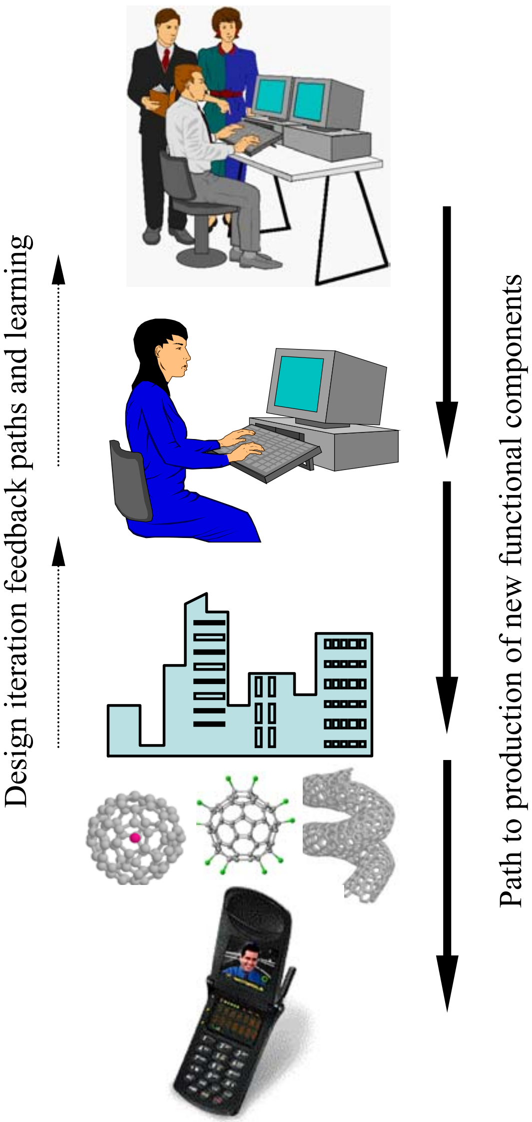


- Quadrumers:  $E = \pm 2t - t', t', t'$



- ***Break symmetry*** **to achieve target density of states**
  - **In dilute limit use asymmetric molecular building blocks**

Vision for future device synthesis: System function *made to order* in nano-factories



- **System needs**
  - Specification of required response function
- **Device synthesis tools for quantum systems**
  - Translation of specifications into physical constraints
  - Search and optimization of actual response relative to target response
- **Nano-factory**
  - Fabrication of *non-intuitive* device designs using structures with nano- and atomic scale tolerance
- **Functional system components**
  - Delivery and integration of functional components to system user

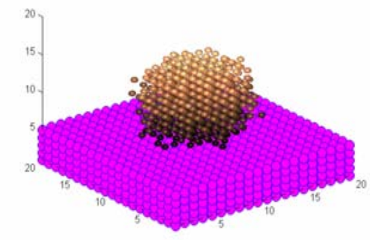
Example of more sophisticated physical model: Linear response of inhomogeneous media, $\varepsilon(\mathbf{r},\mathbf{r}',\omega)=\varepsilon_{\mathrm{ph}}(\mathbf{r},\mathbf{r}',\omega)+\chi_{\mathrm{el}}(\mathbf{r},\mathbf{r}',\omega)$

- **Assume positive jellium background. Potential, *V*(r), and** $\varepsilon_{\mathrm{ph}}(\mathbf{r},\mathbf{r}',\omega)=\varepsilon_{\mathrm{ph}}(\omega)$
- **Solve Schrödinger equation for unperturbed system of non-interacting electrons**

$$H_0=-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})$$

- **Linear response theory (the induced charge density is linearly proportional to the total potential)**

$$\phi_{\mathrm{tot}}(\mathbf{r})=\phi_{\mathrm{ext}}(\mathbf{r})+\phi_{\mathrm{ind}}(\mathbf{r})$$

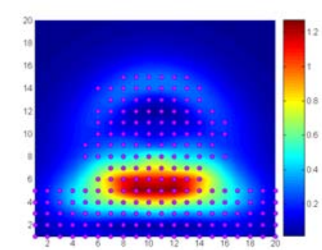


- **The induced potential satisfies Poisson equation:**

$$\nabla^2\phi_{\mathrm{ind}}(\mathbf{r})=4\pi\rho_{\mathrm{ind}}(\mathbf{r}) \qquad \phi_{\mathrm{ind}}(\mathbf{r})=\int_V\frac{\rho_{\mathrm{ind}}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}'$$

- **Calculation of induced charge density (within the linear response approximation):**

$$\rho_{\mathrm{ind}}(\mathbf{r}')=\int_V\chi_{\mathrm{el}}(\mathbf{r}',\mathbf{r}'',\omega)\phi_{\mathrm{tot}}(\mathbf{r}'')d^3\mathbf{r}''$$



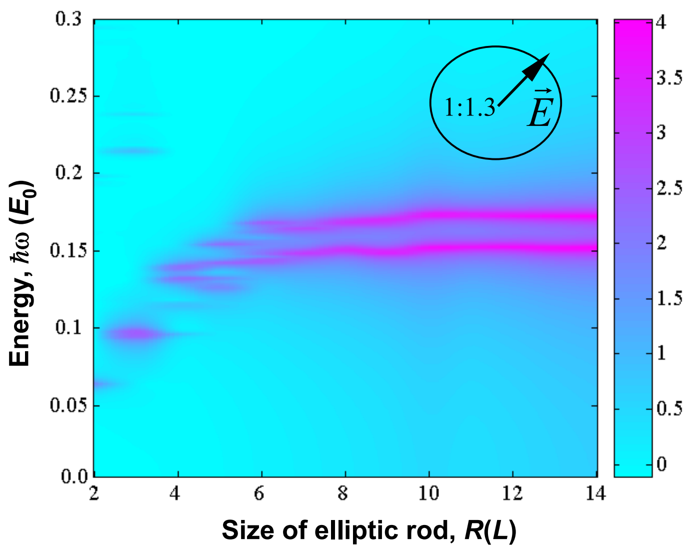
- **Non-local density-density electron response function using RPA :**

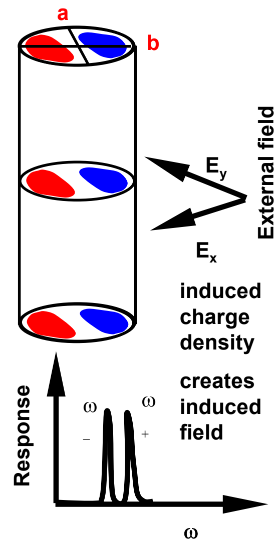
$$\chi_{\mathrm{el}}(\mathbf{r},\mathbf{r}',\omega)=\sum_{i,j}\frac{f(E_i)-f(E_j)}{E_i-E_j-\hbar\omega-i\gamma}\psi_i^{(0)}(\mathbf{r})\psi_i^{(0)}(\mathbf{r}')\psi_j^{(0)*}(\mathbf{r})\psi_j^{(0)}(\mathbf{r}')$$

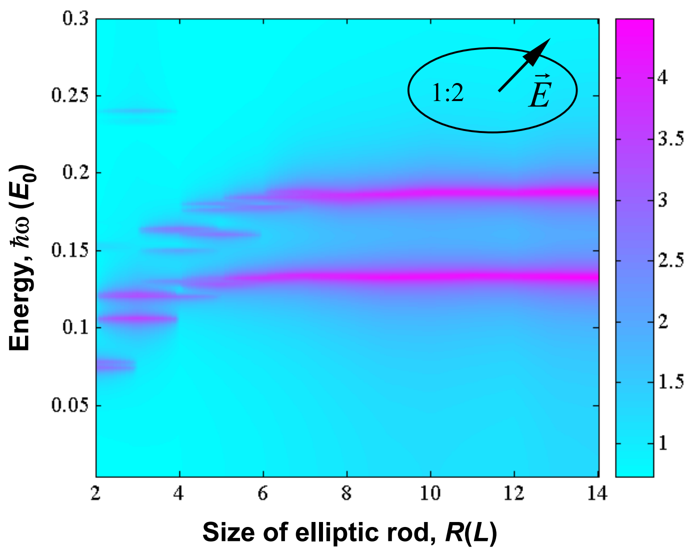
- **Self-consistent integral equation for the induced potential**

$$\boxed{\phi_{\mathrm{ind}}(\mathbf{r})=\sum_{i,j}\frac{f(E_i)-f(E_j)}{E_i-E_j-\hbar\omega-i\gamma}\int_V\frac{\psi_i^*(\mathbf{r}')\psi_j(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}'\int_V\psi_j^*(\mathbf{r}'')(\phi_{\mathrm{ext}}(\mathbf{r}'')+\phi_{\mathrm{ind}}(\mathbf{r}''))\psi_i(\mathbf{r}'')d^3\mathbf{r}''}$$

Size-effects for linear dielectric response of elliptic rod: The classical-quantum boundary for nano-metla light interaction





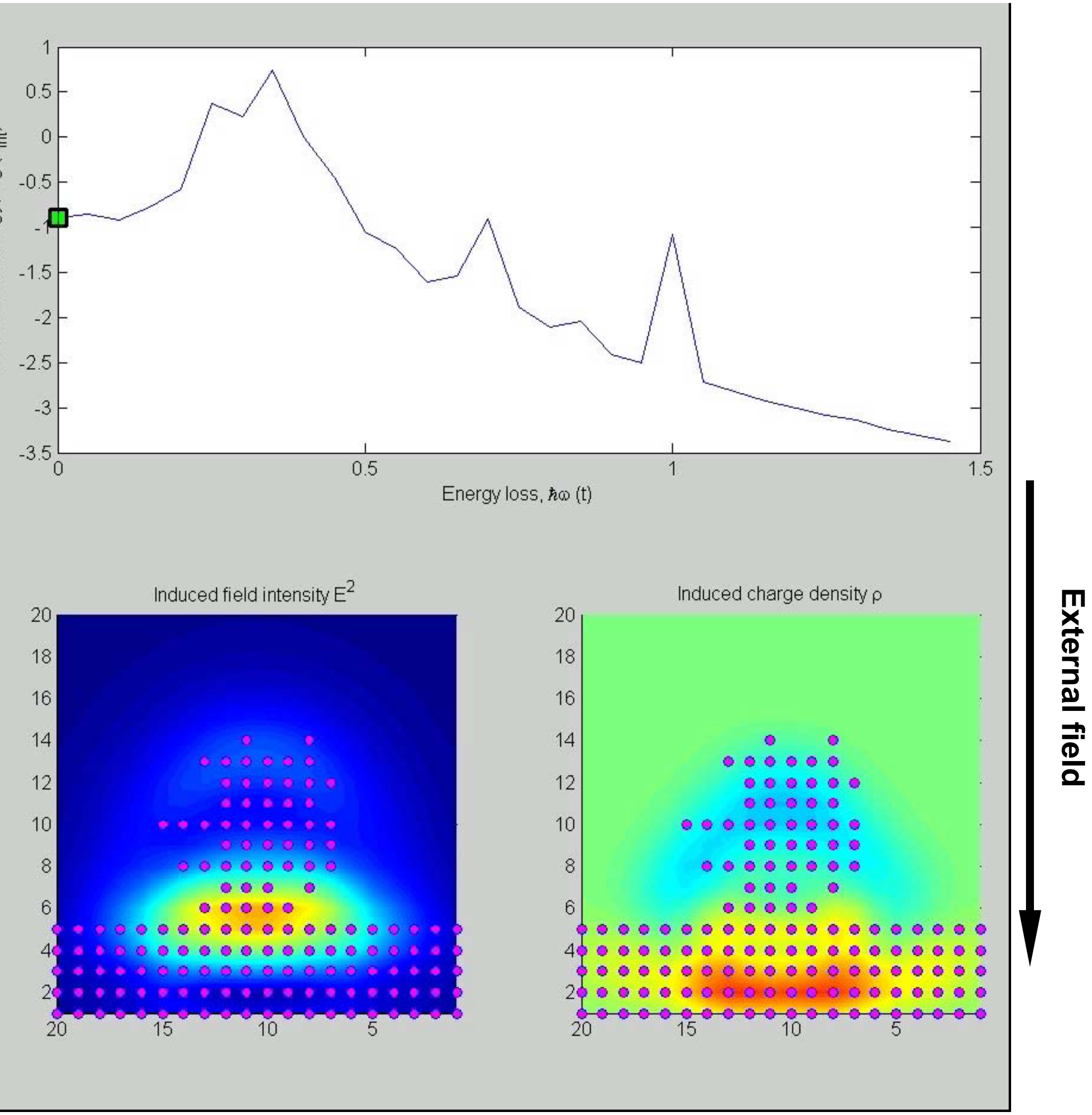


- **Elliptic cylinder with semi-axis *a* and *b* where $x^2/a^2 + y^2/b^2 = R^2$ and $a < b$. Periodic boundary conditions in *z* direction**
- **Energy of induced electric field W_{ind} in elliptic rod as a function of field frequency ω and R**

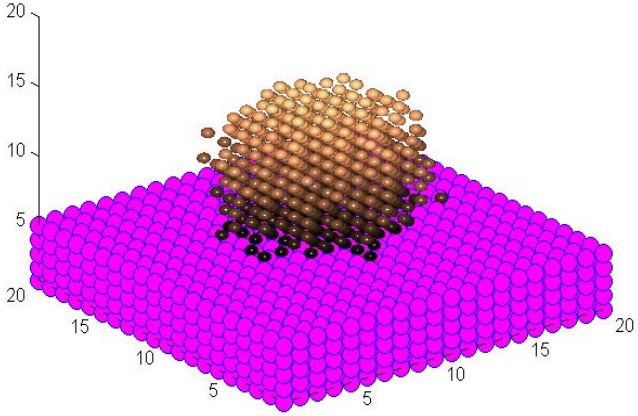
$$\boxed{W_{ind} \propto \int_V \left|\vec{\mathrm{E}}_{\mathrm{ind}}\right|^2 d^3\vec{r}}$$

- **Aspect ratios a:b = 1:1.3, and a:b = 1:2, classical Mie plasmon frequencies $\omega^+ = \omega_p(b/(a+b))^{1/2}$ and $\omega^- = \omega_p(a/(a+b))^{1/2}$ where $\omega_p = (4\pi e^2\rho/m)^{1/2}$**
- **GaAs, $\rho = 10^{18}$ cm^{-3}, L = 1.28 nm, $E_0 = \hbar^2/2mL^2$ = 330 meV, $\gamma = 10^{-3}$, T = 0 K**
- **For R < 6 *L* quantum finite size effects control dielectric response**
- **Collective excitation phase velocity larger than Fermi velocity**
- **Spectral strength at lower frequencies for smaller *L* due to anharmonicity of the jellium potential**

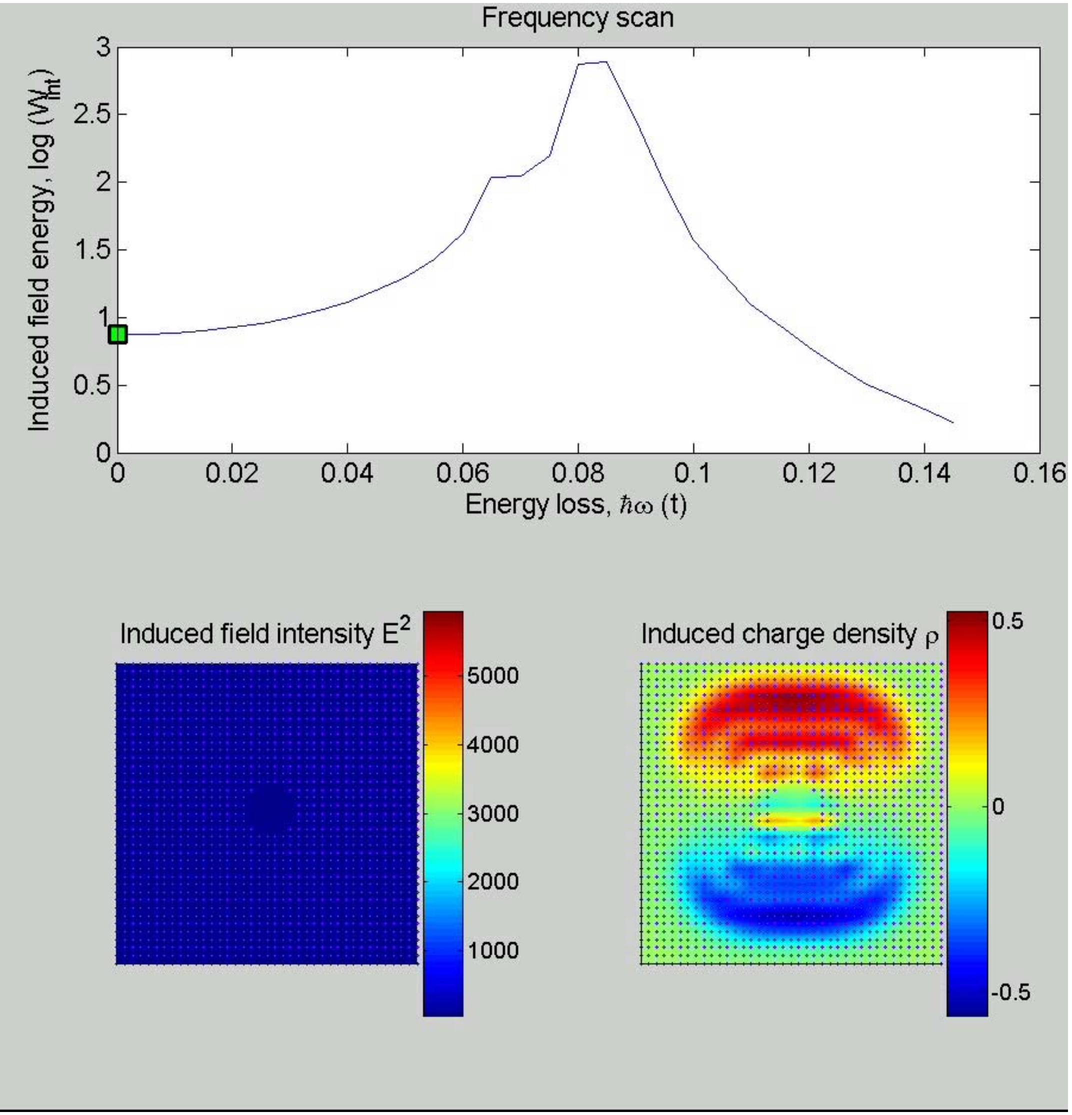
Frequency response of rough nanoparticle on a surface



- **Random number generator used for particle roughness**
- **Electromagnetic field enhancement via resonances**
  - **Sub-wavelength focusing**
  - **Local field enhancement**
- **Control of electromagnetic field enhancement possible using optimal configuration of multiple particles**
  - **The *coexistence of classical and quantum response* create additional degrees of freedom**

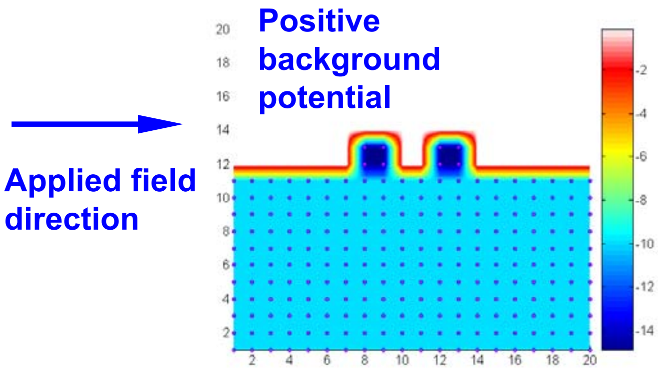


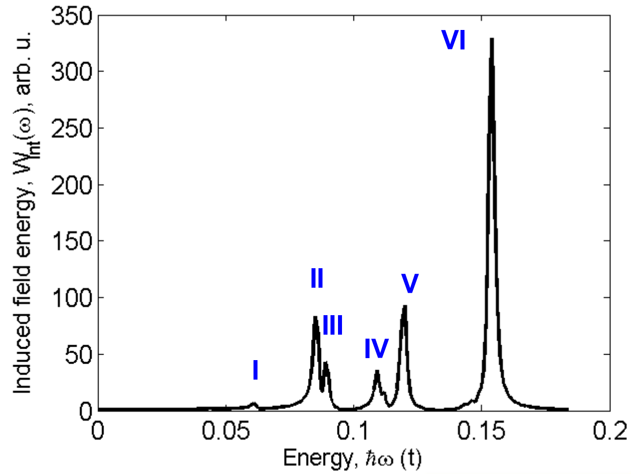
Plasmon-induced sub-wavelength light transmission



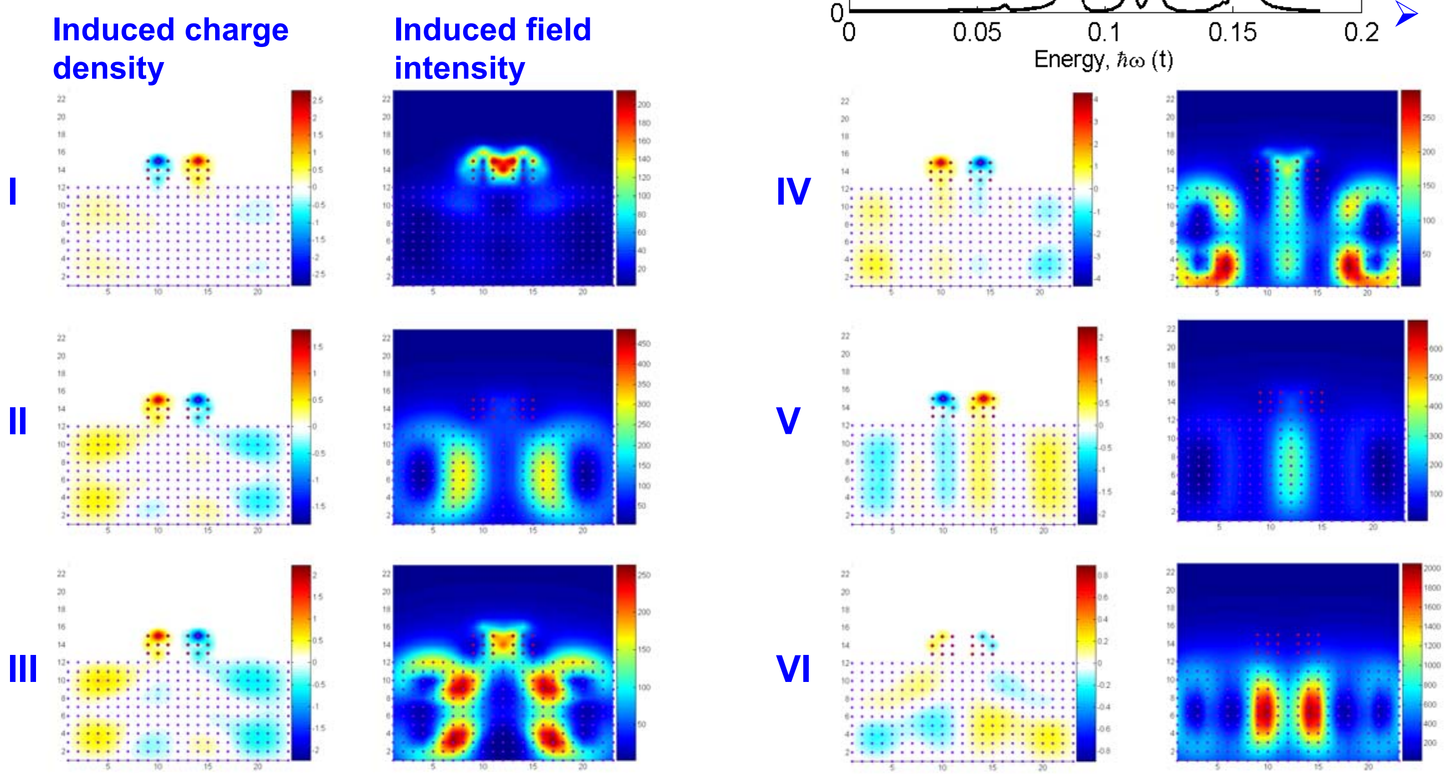
- **Plasmon-enhanced light penetration of sub-wavelength diameter hole**
  - **Enhancement in transmission is about 2 orders of magnitude**
- **Control of electromagnetic field penetration possible using optimal spatial configuration**
  - **The coexistence of classical and quantum response create additional degrees of freedom**
- **Parameters**
  - **Number of electrons in the system: *N* = 126**
  - **Dimension of the metal foil: 60x60x16**
  - **Radius of hole *R* = 4*L***
- ***All* previous calculations use idealized geometry and idealized or phenomenological description of dielectric response**
  - H.A. Bethe, Phys. Rev. **66**, 163 (1944)
  - Schatz, Optics Express **13**, 3150 (2005)

Optical excitation of diatomic molecule on surface of metal grain





- Multiple peaks and shifts in frequency spectrum due to metal – molecule interaction
- Molecule signature peak I, III, IV
- Strongest spectral features come from metal grain
  - Larger density of states
- $t = \hbar^2/2mL^2$



Quantum transport in electronic devices

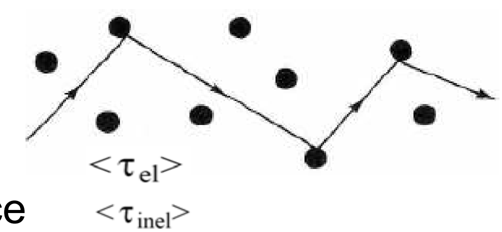
- **Nanoscale electronic devices using optimal design**
  - Self-consistent Schrödinger - Poisson solver required
    - Schrödinger equation $\hat{H}\psi = E\psi$
      - Time dependent Schrödinger equation $\hat{H}\psi = i\hbar\partial_t\psi$
    - Poisson equation $\nabla^2\phi = -\rho/\varepsilon$
      - Maxwell equations
- **Prototype problem is modification of conduction band profile to create linear current-voltage characteristic in presence of ballistic transport and tunneling**
  - Can inherent nonlinear transfer characteristics and exponential sensitivity in nanoscale devices be suppressed?
- **Exhaustive search methods to be used and then compared quantitatively with other approximate methods**
  - Efficient optimizers for electronic devices

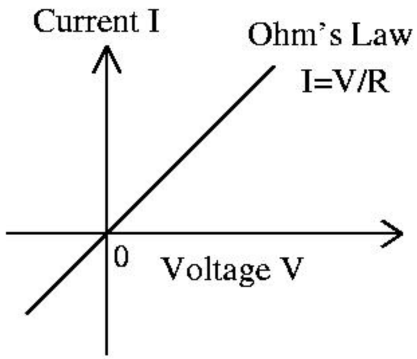
Example: Quantum transport in electronic devices

- **Prototype problem is modification of conduction band profile to create linear current-voltage characteristic in presence of ballistic transport and tunneling**
  - **Can inherent nonlinear transfer characteristics and exponential sensitivity in nanoscale devices be suppressed?**

Ohm's law:

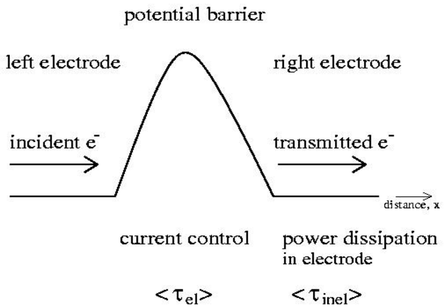
- Diffusive electron transport
- Conduction limited by electron dissipation/scattering
- $<\tau_{el}>$, $<\tau_{inel}>$ over same region of space

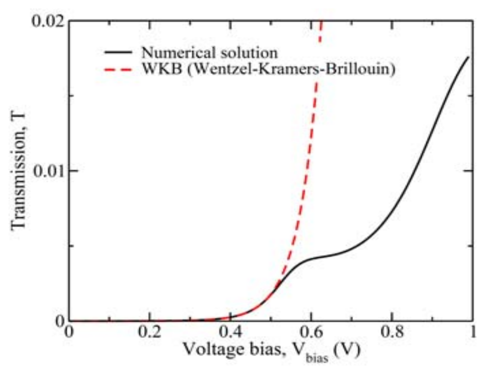




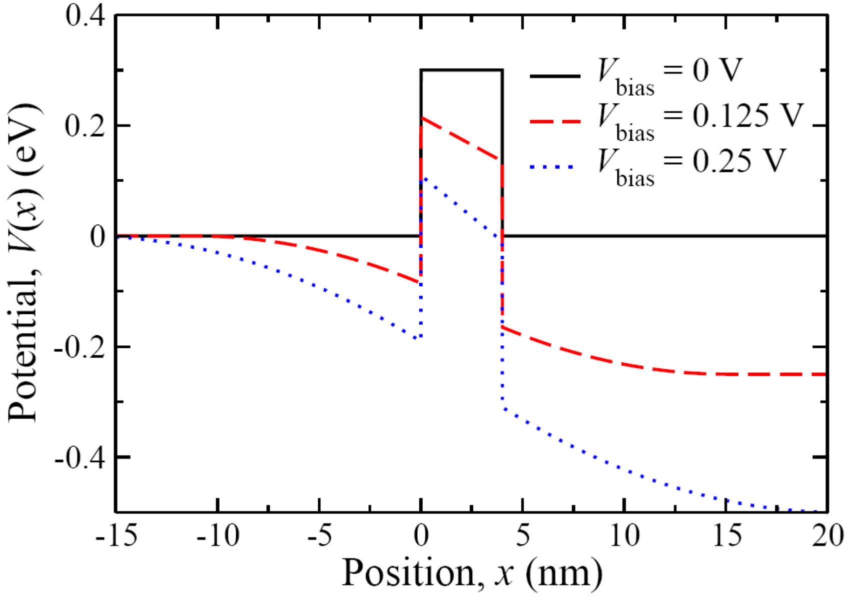
Electronic nanoscale semiconductor device:

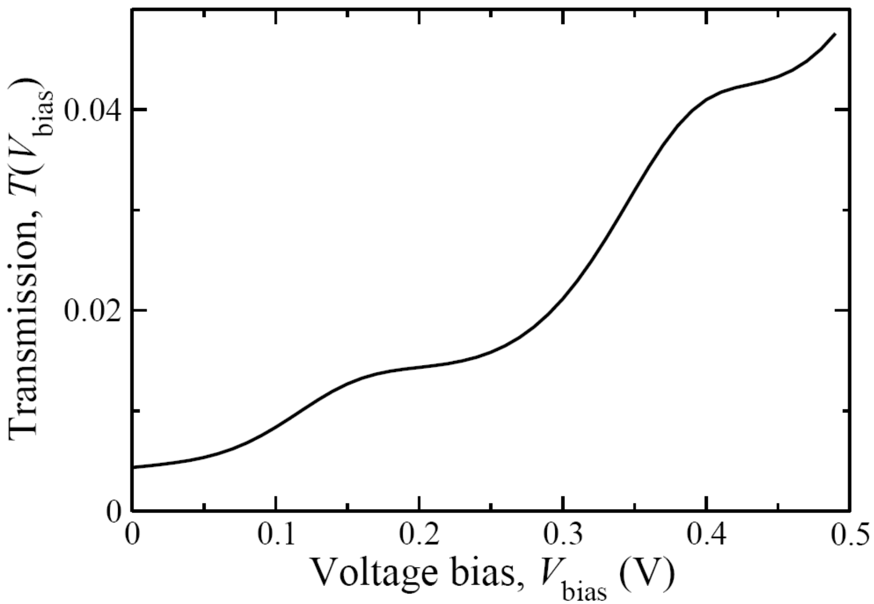
- Ballistic electron transport
- Exquisite current control in potential barrier, limited by quantum mechanical transmission
- $<\tau_{el}>$, $<\tau_{inel}>$ spatially separated





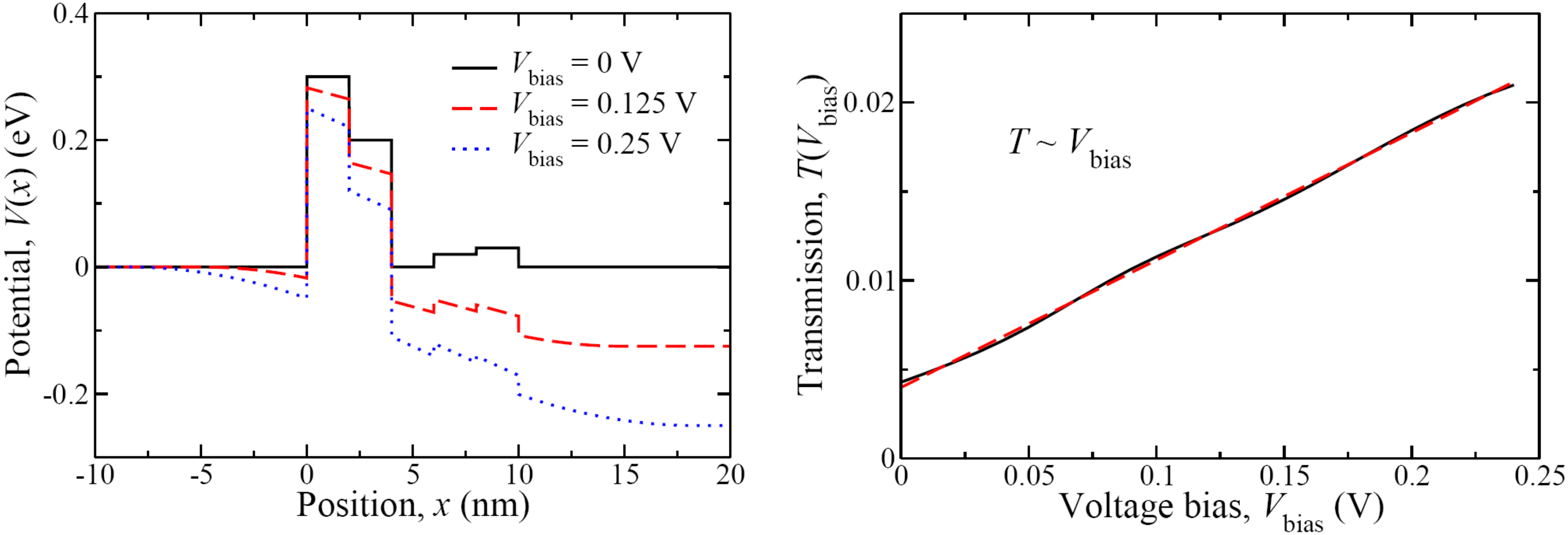
Electron transmission-voltage characteristic





- Rectangular barrier 0.3 eV energy ($Al_xGa_{1-x}As$), 4 nm wide
- Electrode carrier concentration is $n = 10^{18}$ cm^{-3}
- Effective electron mass $m^* = 0.07 \times m_0$ (GaAs)
- Incident electron energy E = 26 meV
- Solve Schrödinger equation in piecewise fashion using propagation matrix and calculate transmission $T(V_{bias})$
- Use Poisson equation to calculate band bending at V_{bias}

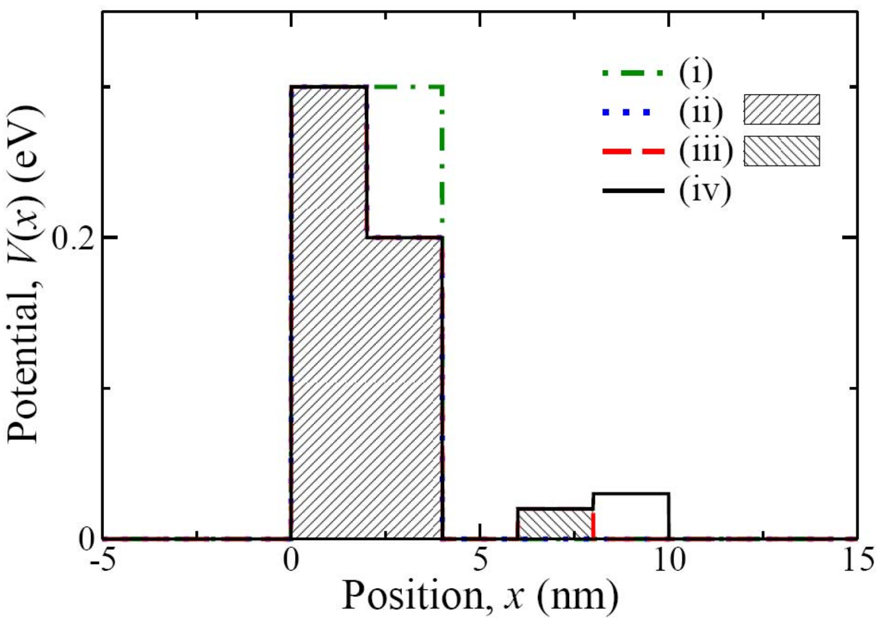
Example: Best potential profile with linear transmission voltage found using exhaustive search

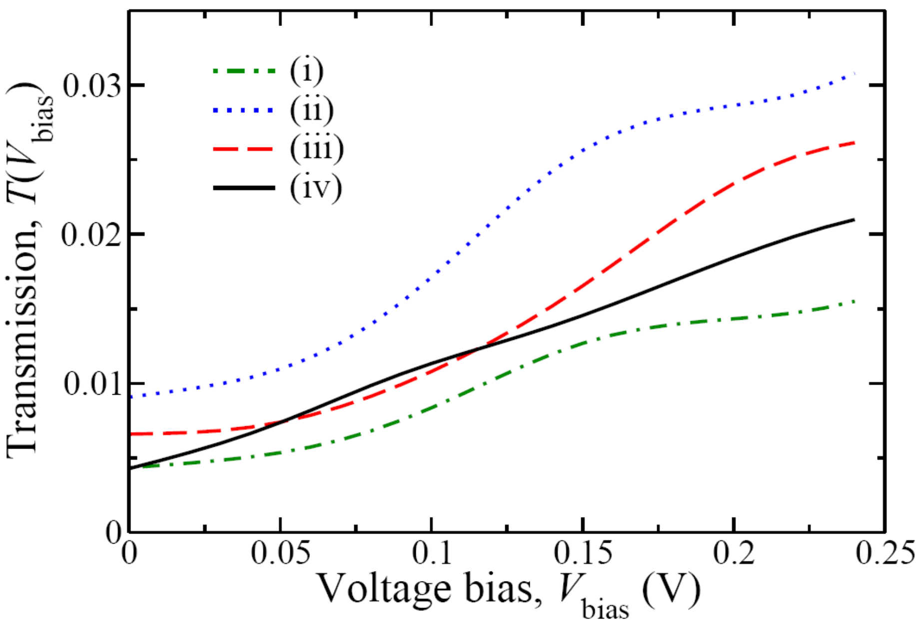


- **Non-intuitive potential profile, *V*(*x*)**
  - **Exhaustive search on grid with Δx = 2 nm (8 monolayer GaAs), ΔV = 0.01 eV.**
  - **Maximum on-site potential 0.3 eV, total width 10 nm, incident electron energy *E* = 26 meV**
  - **Quadratic deviation from linear transmission:** $\chi^2 = 5.1 \times 10^{-7}$

$$\chi^2 = \frac{\sum_{V_{\text{bias}}} \left(J\left(V_{\text{bias}}\right) - J_0\left(V_{\text{bias}}\right)\right)^2}{\sum_{V_{\text{bias}}} \left(J\left(V_{\text{bias}}\right)\right)^2}$$

Understanding the physics: Evolution from single barrier (i) to optimal potential profile

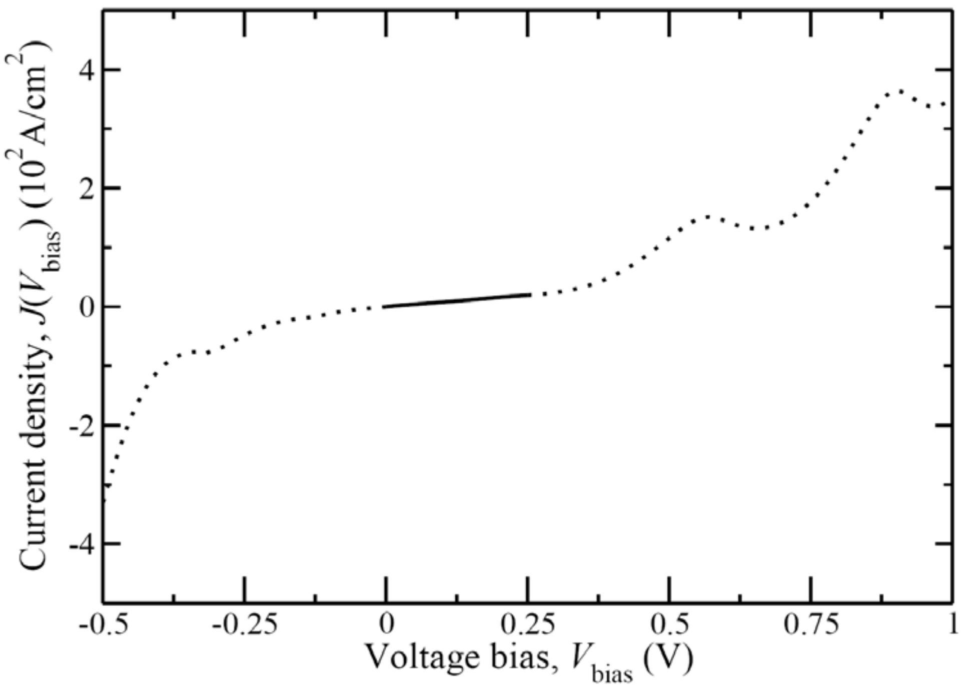


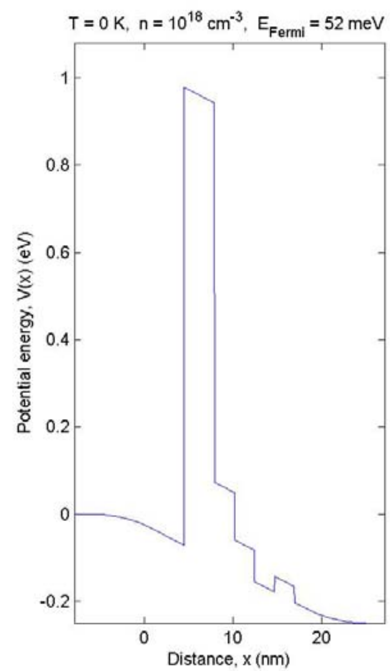


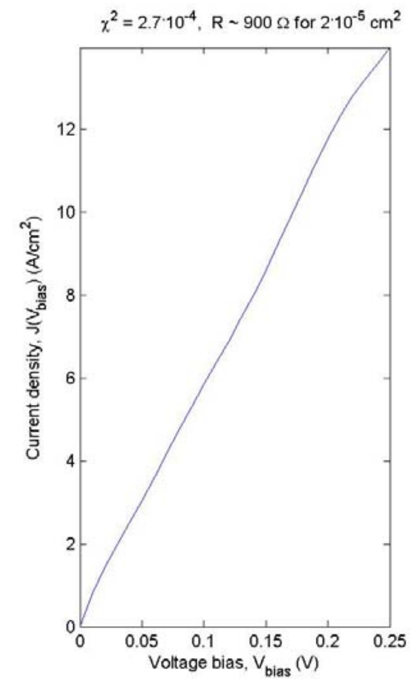
- **Superposition of broad scattering resonances from different potential steps results in linear transmission-voltage curve**
- **Control of pole energy and strength determines transfer function**
- **Insensitivity to monolayer variations in potential and robustness of design associated with broadness of resonances**

Quantum electron transport: Non-intuitive design

- **Synthesis of current voltage characteristics in semiconductor devices**
  - **Machine generated non-intuitive conduction band potential profile for linear current-voltage characteristics from 0 V to 0.25 V**
    - **Current state-of-the-art limited to elastic scattering only**
      - **Future physical model development to include inelastic processes**
      - **Future integration with optimizer**

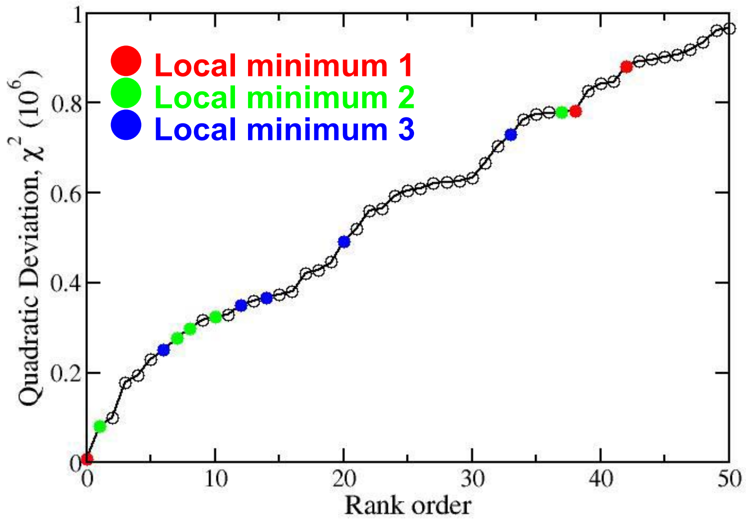


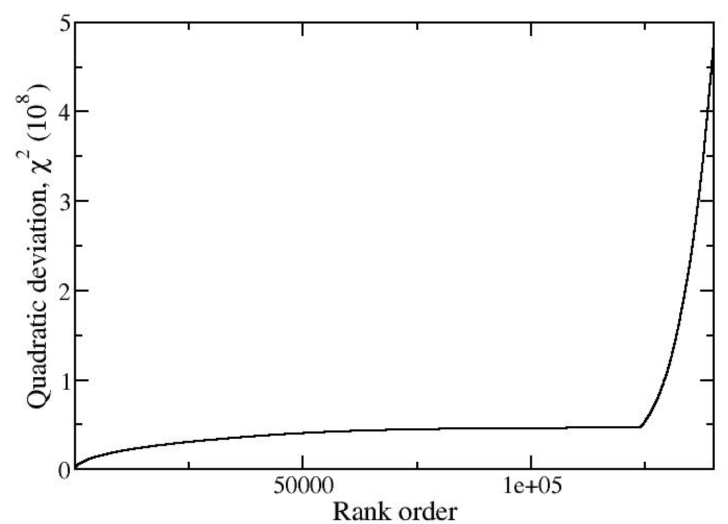




Combining exhaustive search with adjoint method

- **Exhaustive search among all potentials on a specified discrete grid in space and potential energy:**
  - **Δx = 4 monolayers, where a monolayer in GaAs is 0.282665 nm**
  - **ΔV = 0.036062 eV, corresponds to Al - concentration x = 0.04 in $GaAs/Al_xGa_{1-x}As$ conduction band heterojunction**
  - **Number of barriers = 5, V(x) = 0 ... 5 ΔV**
- **Target function is transmission-voltage characteristic for which V(1) = 2 ΔV, V(2) = 10 ΔV, V(3) = ΔV, V(4) = 0.0eV, V(5) = ΔV**
  - **Take each of the best 50 potentials as an initial choice and then calculate the local minimum using adjoint method and FMINCON to identify *basins of convergence***
- **Potentials from grid-based exhaustive search converge to different local minima (different colored dots)**
  - **Non-convex solution space**

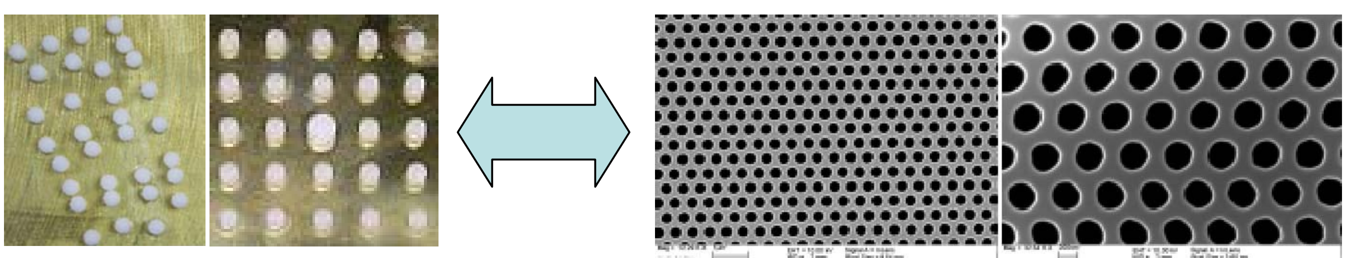




Aperiodic dielectric design

- **Goal**
  - Verify experimentally device synthesis tools and methodology
  - mm-wave (37.5 GHz, λ_0 = 8 mm) test-bed
    - Rapid prototyping, high tolerance control (±2μm / λ_0 = 1/4000), relatively low cost
      - Compare with achievable tolerance for nanophotonics which is Λ = 500 nm, ±5 nm / Λ = 1/100
    - Solve Helmholtz equation $\partial_x \frac{\mu_0}{\mu_y} \partial_x \boldsymbol{E} + \partial_y \frac{\mu_0}{\mu_x} \partial_y \boldsymbol{E} + \omega^2 \mu_0 \varepsilon_0 \varepsilon_{\mathrm{rel}} \cdot \boldsymbol{E} = 0$
      - FDFD
      - Interior boundary is TE10 mode at wave guide aperture
      - In modeling domain μ_r = 1 and $\varepsilon_r = \varepsilon_r(x, y)$ varies discontinuously at cylinder boundary
  - Meet top-hat design metrics
    - 30 dB side lobe suppression, ±0.15 dB ripple, 90% coupling
  - Develop efficient robust optimization design tools
    - Local optimization using adjoint method
    - Global optimization, heuristic rule-based method, interactive visualization
  - Generalized methodology
    - High dimensionality of design space, nonlinearity, non-convexity
    - Exponential sensitivity, optimization without single objective function

mm-wave



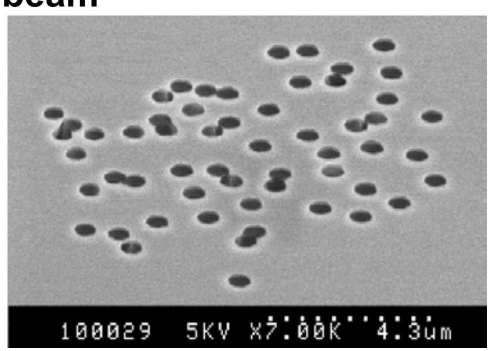
Nano-photonic

Aperiodic nano-photonics: *Uniform* illumination of a surface

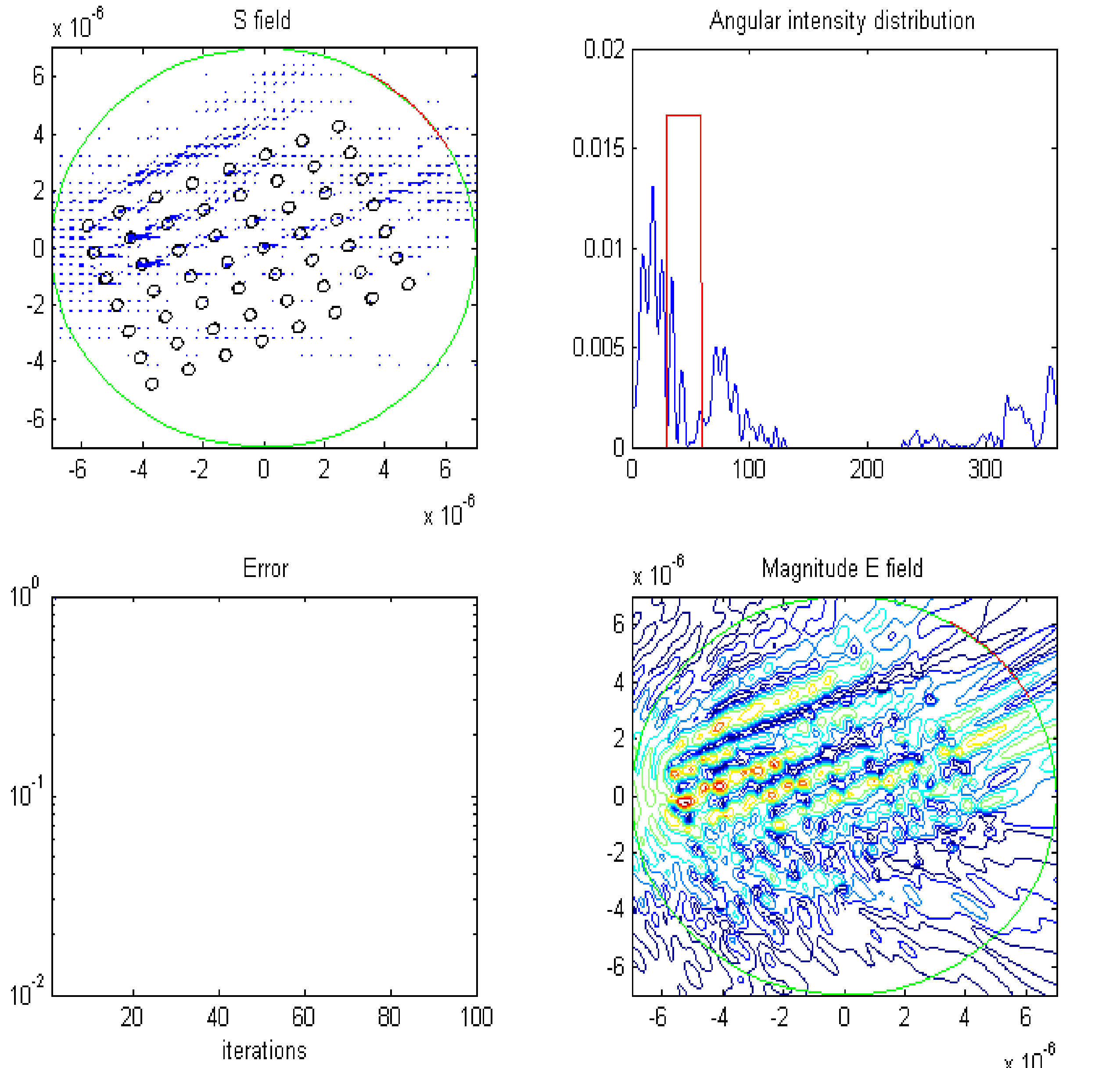
New generation of broken symmetry nano-photonics devices

56 dielectric scattering centers configured to convert gaussian profile input beam of width $2\sigma = 4$ μm into 30° – 60° top hat intensity function at 7 μm radius observation circle

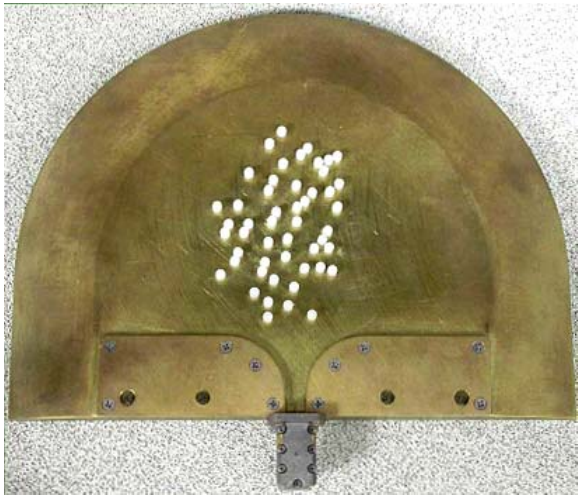
Size of aperiodic nano-photonic structure dominated by size of input beam



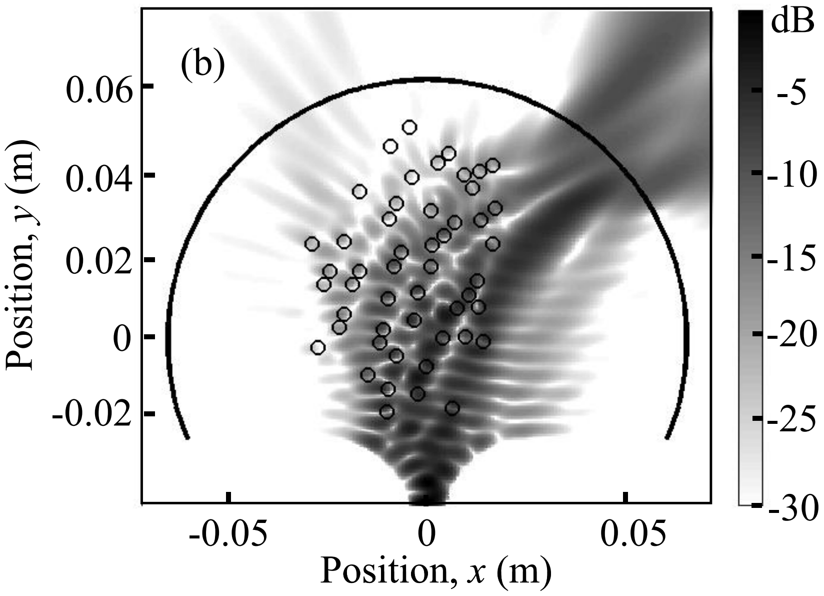
Aperiodic nano-photonic design patterned using e-beam lithography in Si slab waveguide geometry

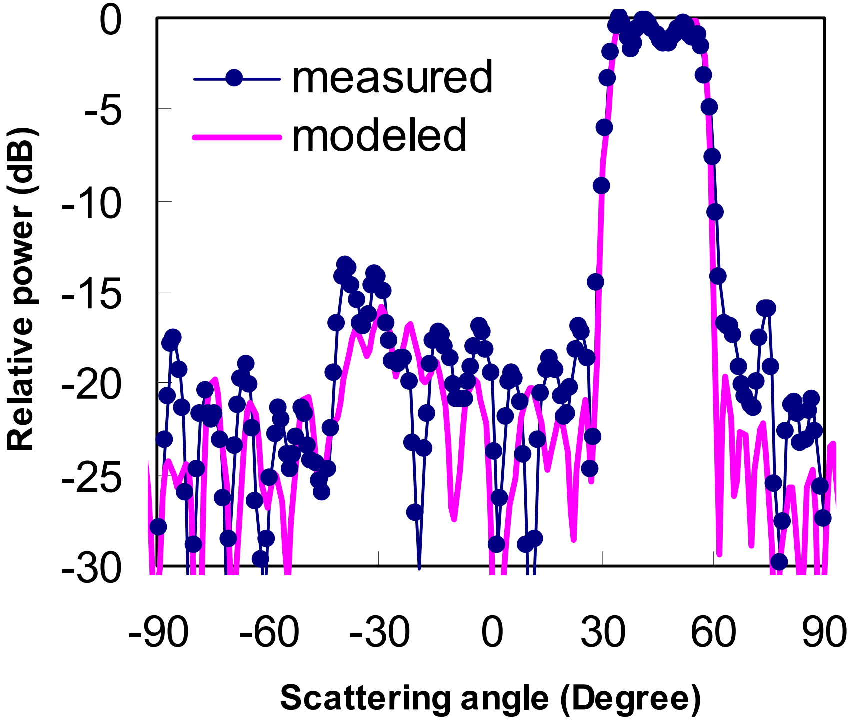


Aperiodic electromagnetic design: Experimental verification of uniform illumination between 30° and 60° scattering angles



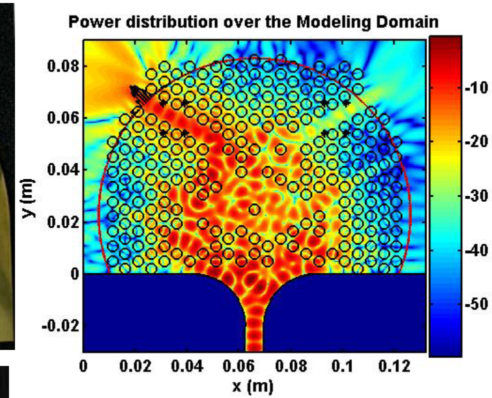
- **Adjoint method**
- **Good agreement between model and measured data at 37.5 GHz (λ_0 = 8 mm)**
  - **95% calculated, 92.4% measured power uniformly illuminates between 30° and 60° scattering angles**
  - **±0.725 dB calculated, ±0.885 dB measured ripple in illuminated power between 30° and 60° scattering angles**

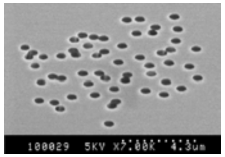


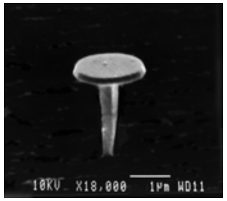


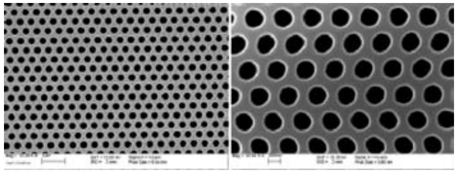
Nanophotonic and RF design

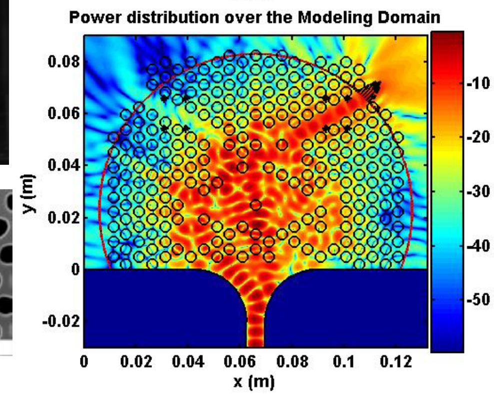
- **Aperiodic arrangements of dielectrics and metals for filters and micro-spectrometers**
  - **Synthesis for *non-intuitive* design**
    - **Compact WDM filter and spectrometer for chip-scale photonics**
- **Exploration for new functionality**
  - **Accessibility of scaled nanophotonic devices**
    - **Room-temperature operation of λ_0^3 volume laser diode**
    - **Single photon source at λ_0=1550 nm or λ_0=850 nm**
    - **Lasing based on Si materials**
  - **New configurations using negative index material for unique behavior and performance**
    - **Discovery of performance metrics for new building blocks such as resonators and lenses**
- **Optimal design of negative index physical media**
  - **Optimized meta-materials**
    - **Metal and dielectric configurations with low dispersion and low losses at RF and optical frequencies**

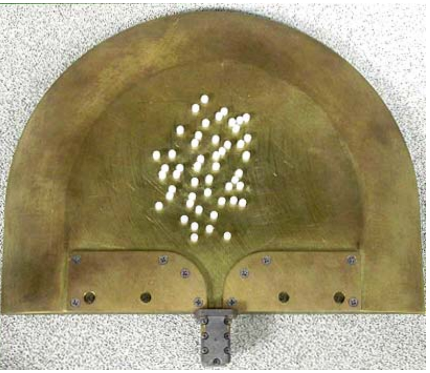


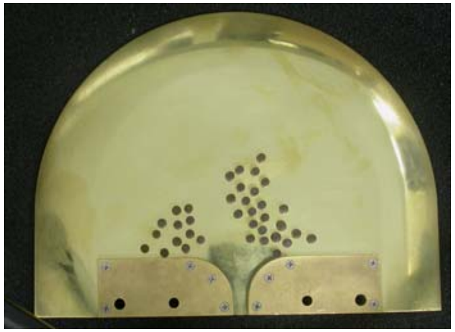


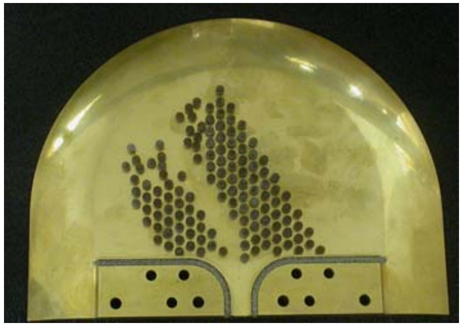


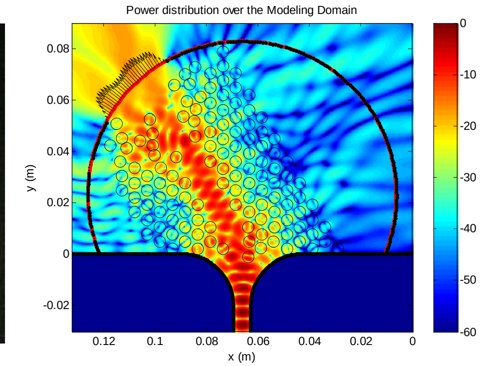






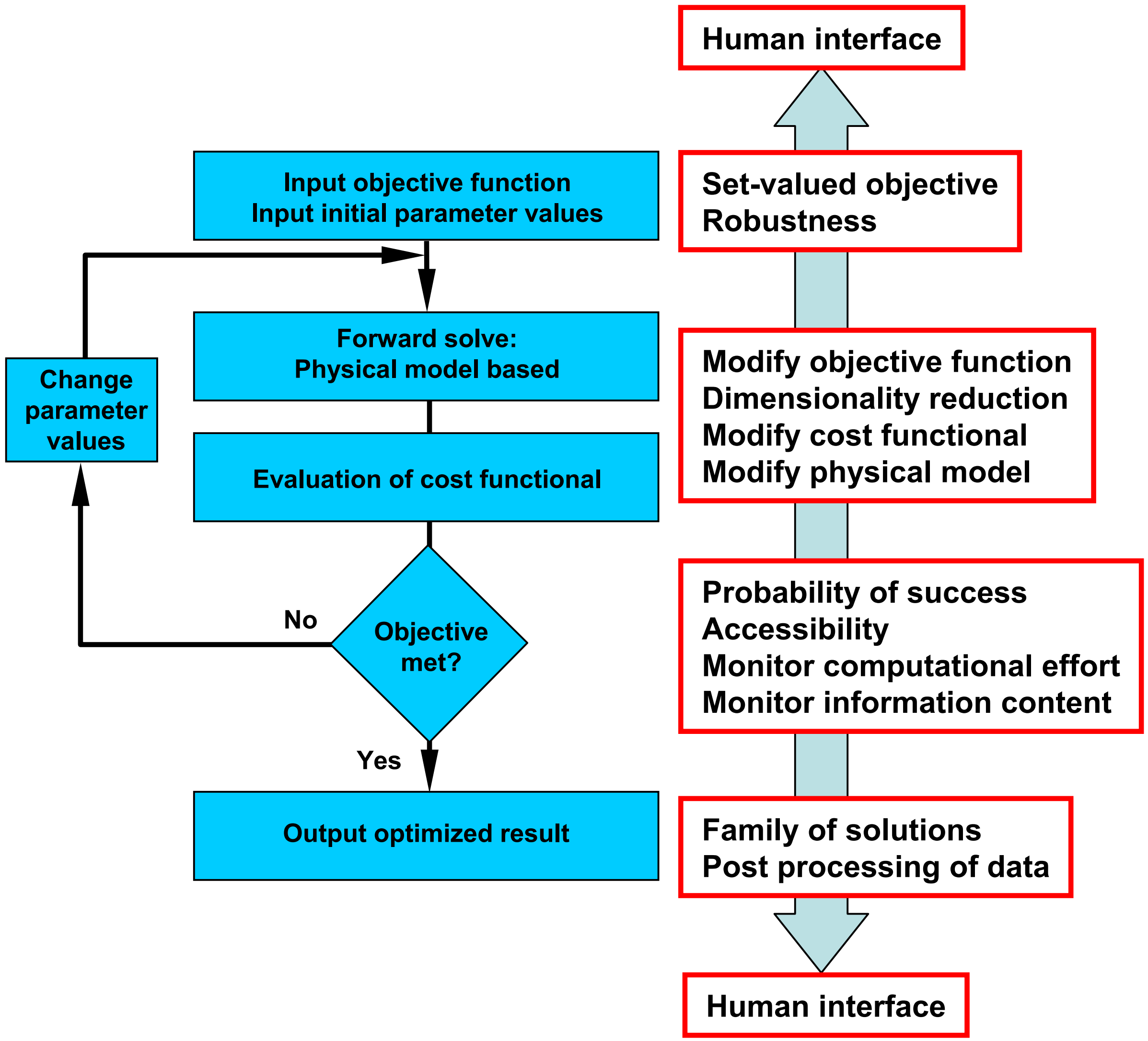




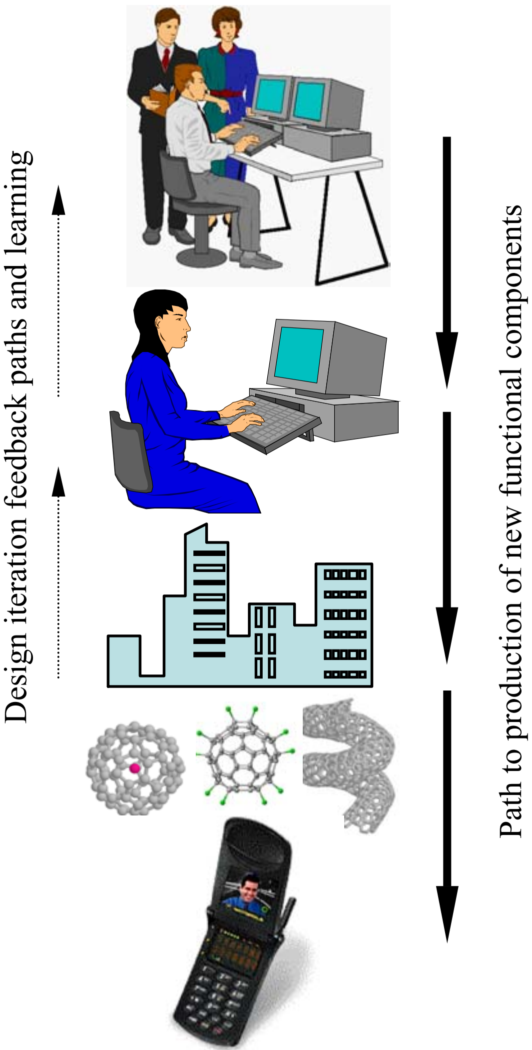


Adaptive optimization concept

- Conventional approach
  - Objective function
  - Cost functional
  - Forward solve and iterate
- Intelligent optimization
  - Maximally exploit available information with minimum effort
  - Significant adaptive control loops within and between modules
  - Interactive
- At end of computation both problem and algorithm have changed
  - *Adaptive optimization*
- Automatically discover extreme physical behavior of nano-scale inhomogeneous configurations using first-principles calculations of light-matter interactions
  - Linear scaling DFT
  - Quantized electromagnetic field

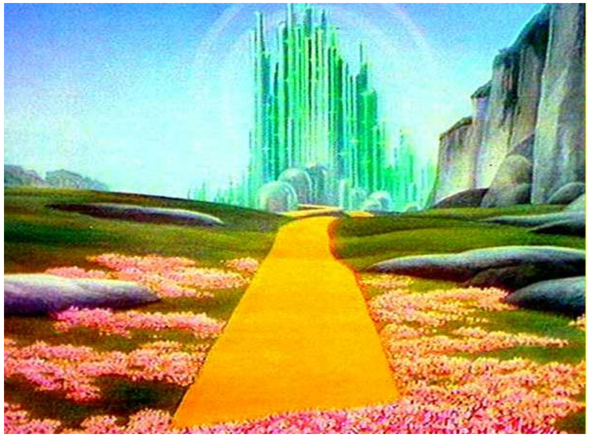


Requirements for system function *made to order*



- **Efficient**
  - ***Realistic* physical models**
  - ***Adaptive* optimization**
  - ***Human* interaction for learning (real time)**
- **System needs**
  - **Specification of required response function**
- **Device synthesis tools for quantum systems**
  - **Translation of specifications into physical constraints**
  - **Search and optimization of actual response relative to target response**
- **Nano-factory**
  - **Fabrication of *non-intuitive* device designs using structures with nano- and atomic scale tolerance**
- **Functional system components**
  - **Delivery and integration of functional components to system user**

Securing systems beyond Moore's Law endpoint in 2020



The semiconductor industry technology roadmap

When the road turns to dirt, the dinosaurs die

with

Ultimate Technology

Nano-metal
Ilya Grigorenko
Stephan Haas
Electron transport
Petra Schmidt
Gary Rosen
Aperiodic design
Chunming Wang
Philip Seliger