nextnano
Software for semiconductor nanodevices

nextnano Workshop

- **pn junction**
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_pn_junction.htm
  `GaAs_pn_junction_1D*.in` (nextnano++ & nextnano^3)
  `GaAs_pn_junction_2D*.in` (nextnano++ & nextnano^3)
  This example is rather simple. ➔ Poisson equation
  Try to reproduce the results in the figures. Run and plot the 2D files.
  Challenge: To plot two different graphs, i.e. data files, simultaneously. Export the graph containing two different graphs to gnuplot. Export a 2D file to gnuplot.
  (10 minutes)

- **(Important)**
  Schrödinger-Poisson - A comparison to the tutorial file of Greg Snider's code
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_SchroedingerPoisson.htm
  `Greg_Snider_MANUAL_1D_*.in` (nextnano++ & nextnano^3)
  This example is relatively easy. ➔ self-consistent Schrödinger-Poisson
  Try to reproduce the results in the figures.
  Challenge: To plot two different graphs, i.e. data files, simultaneously.
  Understand where you find eigenvalues and wavefunctions. Export the graph containing two different graphs to gnuplot.
  (20 minutes)

- **(Important)**
  Double Quantum Well
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_DoubleQW.htm
  `DoubleQuantumWell_6nm_nnp_*.in` (nextnano++ & nextnano^3)
  This example teaches quantum physics: bonding and anti-bonding wavefunctions.
  ➔ Schrödinger-equation
  Try to reproduce the results in the figures.
  Challenge: Perform a parameter sweep using nextnanomat's **Template** feature and do a post-processing using nextnanomat to reproduce the figure "Eigenvalues vs. barrier width". Export the graph to gnuplot.
  (20 minutes)

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- **Optical interband transitions in a quantum well - Matrix elements and selection rules**
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_OpticalTransitions.htm
  `1DQW_interband_matrixelements__*.in` (nextnano++ & nextnano^3)
  This example teaches how to calculate the spatial overlap of electron and hole wavefunctions and their transition energy.
  Challenge: Compare the infinite vs. finite quantum well to understand selection rules.
  (10 minutes)

- **Wurtzite**
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial11.htm
  `wurtzite_*.in` (nextnano++ & nextnano^3)
  This example is relatively easy and discusses strain, piezo any pyroelectricity. ➔ Strain & Poisson equation
  Try to reproduce the results in the figures.
  Challenge: To understand the peculiarities of wurtzite.
  (20 minutes)

- **Two-dimensional electron gas in an AlGaN/GaN field effect transistor**
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_AlGaN_GaN_FET.htm
  `Jogai_AlGaNGaN_FET_JAP2003_*.in` (nextnano++ & nextnano^3)
  This example is nice.
  Try to reproduce some of the figures.
  Challenge: Can you do a parameter sweep using nextnanomat's Template feature and plot the 2DEG density vs. $Al_xGa_{1-x}N$ thickness?
  (20 minutes)

- (Advanced)
  (Important)
  k.p dispersion in bulk GaAs (strained / unstrained)
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial13.htm
  `bulk_kp_dispersion_GaAs__*.in` (nextnano++ & nextnano^3)
  This example teaches the k.p band structure.
  Try to reproduce some of the figures: Plot the single-band, the 6-band dispersion and the 8-band E(k) dispersion in the same plot. Do the same for the strained case to see how strain alters the band structure.
  Challenge: To understand the k.p method.
  (15 minutes)

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k.p dispersion in bulk unstrained ZnS, CdS, CdSe and ZnO (wurtzite)
https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_bulk_6x6kp_dispersion_IIVI.htm
`bulk_6x6kp_dispersion_ZnO_*.in` (nextnano++ & nextnano^3)
This example teaches the k.p valence band structure for wurtzite materials.
(5 minutes)

k.p dispersion in bulk unstrained, compressively and tensilely strained GaN (wurtzite)
https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_strained_GaN_dispersion.htm
`bulk_kp_dispersion_GaN_unstrained_*.in` (nextnano^3)
This example teaches the k.p valence band structure for wurtzite materials.
(10 minutes)

- (Advanced)
  (Important)
  Energy dispersion of holes in a quantum well
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial8.htm
  `1Dwell_GaAs_AlAs_nn3_*.in` (nextnano++ & nextnano^3)
  This example teaches the k.p model: E($k_{||}$) dispersion
  Try to reproduce some of the figures.
  Challenge: To understand the k.p features.
  (20 minutes)

- (Advanced)
  (Important)
  k.p dispersion of an unstrained GaN QW embedded between strained AlGaN layers
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_GaN_AlGaN_QW_dispersion.htm
  `1DGaN_AlGaN_QW_k_zero*.in` (nextnano++ & nextnano^3)
  This example teaches the k.p model: E($k_{||}$) dispersion
  Try to reproduce some of the figures.
  Challenge: To understand the k.p features.
  (20 minutes)

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- (Advanced)
  Capacitance-Voltage curve of a "metal"-insulator-semiconductor (MIS) structure
  https://www.nextnano.com/nextnano3/tutorial/1Dtutorial_MIS_CV.htm
  `1DMIS_CV_Fermi_*.in` (nextnano++ & nextnano^3)
  This example teaches how to apply a bias without solving the current equation. Try to reproduce some of the figures.
  Challenge: To understand how to integrate charge carrier densities in specific regions.
  (20 minutes)

- (Advanced)
  (VERY IMPORTANT)
  InGaAs Multi-Quantum Well Laser diode
  https://www.nextnano.com/dokuwiki/doku.php?id=nnp:1d_ingaas_laser_diode
  `LaserDiode_InGaAs_1D_cl_nnp.in / *_qm.in` (nextnano++)
  This example teaches how to apply a bias and solve the coupled system of Schrödinger, Poisson and Current equations.
  Challenge: To understand how a laser works. Plot the recombination rates and the classical emission spectrum. Do a parameter sweep, e.g. number of wells, doping, alloy content and see how the classical emission spectrum changes. Plot the wavefunctions. Compare the classical density vs. the quantum density for the same bias, e.g. for 1 V where the quantum wells contain a significant density. Plot the convergence log files on a logarithmic scale. Plot the current densities, IV curve, doping profile, …
  (40 minutes)

- (Advanced)
  (Important / 2D example)
  Schrödinger equation of a two-dimensional core-shell structure
  Hexagonal 2DEG - Two-dimensional electron gas in a delta-doped hexagonal shaped GaAs/AlGaAs nanowire heterostructure
  https://www.nextnano.com/nextnano3/tutorial/2Dtutorial_core_shell_circle_hexagon.htm
  `2DGaAs_AlGaAs_nnp_*.in` (nextnano++ & nextnano^3)
  `2D_Hexagonal_Nanowire_2DEG.in` (nextnano++ & nextnano^3)
  This example teaches how to perform a 2D simulation.
  Challenge: To understand how to visualize 2D results and how to export them to gnuplot. Plot the geometry together with the electron density of the modulation doped core-shell nanowire in one graph.
  (15 minutes)

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- (Advanced)
  (Important / 3D example)
  Energy levels in a pyramidal shaped InAs/GaAs quantum dot including strain and piezoelectric fields
  https://www.nextnano.com/nextnano3/tutorial/3Dtutorial_QD_pyramid.htm
  `3DInAsGaAsQDPyramid_PryorPRB1998_10nm_nnp_*.in` (nextnano++ & nextnano^3)
  This example teaches how to calculate and plot strain, piezoelectric charge densities and wavefunctions in a 3D simulation.
  Challenge: To understand how to visualize 3D results and how to export them to Paraview.
  (20 minutes)

- (Advanced)
  (Important / 3D example)
  Single-electron transistor - laterally defined quantum dot
  https://www.nextnano.com/nextnano3/tutorial/3Dtutorial_SET_lateral_QD.htm
  `SET_Scholze_IEEE2000_*.in` (nextnano++ & nextnano^3)
  This example teaches how a gate geometry depletes the 2DEG density locally.
  Challenge: To understand how to visualize 3D results and how to export them to Paraview.
  (15 minutes)

- (Advanced)
  (3D example)
  Quantum dot molecule
  https://www.nextnano.com/nextnano3/tutorial/3Dtutorial_QD_molecule.htm
  3DQD_molecule_cuboid_asymmetric_*.in (nextnano++ & nextnano^3)
  This example teaches how to apply an electric field in a 3D simulation.
  Challenge: To understand how to visualize 3D results and how to export them to Paraview.
  (15 minutes)

- Search through
  - the other input files in the installation folder,
  - the list of tutorials on the website,
  https://www.nextnano.com/nextnano3/tutorial/tutorial.htm
  and simulate the topics that are of interest for you.

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Important nextnanomat features that you should learn

- Tree View vs. List View
- Parameter sweeps using Template
- Parameter sweep post-processing using Template
- Multi-Parameter sweeps using Template (beta)
- Batch list
- Exporting 2D slices of 3D data
- Exporting 1D slices of 2D/3D data
- Export to .vtr
- Exporting 3D data to Paraview
- Open files with notepad++, Origin, …
- Plotting several graphs (Overlay)
- Plotting several graphs in 2D/3D (Overlay)
- New Zoom feature
- SOFT_KILL feature
- Display options
- Tools ➔ Options
- (HTCondor Cloud Computing)
- (In principle you can run also you own software with nextnanomat. nextnanomat can run any executable.)
- How to access online documentation and how is it structured.
- Which features are you missing?

Questions?
Contact support@nextnano.com or stefan.birner@nextnano.com.

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