nextnano++

quick reference to keywords

sth{} is a group — [sth] is a "type"
sth* is required — [sth] is a "choice option"
sth is an attribute — [sth] is an "enum option"

global{}*

- simulate1D{}
- simulate2D{}
- simulate3D{}
- crystal_zb{}
  - x_hkl [int_vec]
  - y_hkl [int_vec]
  - z_hkl [int_vec]
- crystal_wz{}
  - x_hkl [int_vec]
  - y_hkl [int_vec]
  - z_hkl [int_vec]
  - rotation_c_a_ratio_use_substrate [yes, no]
  - rotation_c_a_ratio [real]
- substrate{}*
  - name* [string]
  - alloy_x [real]
  - alloy_y [real]
  - alloy_z [real]
- temperature* [real]
- temperature_dependent_bandgap [yes, no]
- temperature_dependent_lattice [yes, no]
- magnetic_field{}
  - magnetic_field [real_vec_3]
  - strength* [real]
- periodic{}
  - x [yes, no]
  - y [yes, no]
  - z [yes, no]

grid{}*

- xgrid{}, ygrid{}, zgrid{}
  - min_pos [real]
  - max_pos [real]
  - allow_spacing_jumps [yes, no]
  - line{}*
    - pos* [real]
    - spacing* [real]
    - repeat, repeat2{}
      - shift* [real]
      - minus_num [int]
      - num* [int]
    - array, array2{}
      - shift* [real]
      - min [int]
      - max* [int]

structure{}*

- output_region_index{}, output_material_index{}, output_user_index{}, output_contact_index{}, output_alloy_composition{}, output_impurities{}, output_generation{}, output_injection{}
  - boxes [yes, no]
- region{}*
  - repeat_x{}, repeat_y{}, repeat_z{}, repeat2_x{}, repeat2_y{}, repeat2_z{}
    - shift* [real]
    - minus_num [int]
    - num* [int]
  - array_x{}, array_y{}, array_z{}, array2_x{}, array2_y{}, array2_z{}
    - shift* [real]
    - min [int]
    - max* [int]
  - repeat_profiles [alloy, doping, generation, injection, other]
  - everywhere{}
  - line{}
    - x* [real_vec]
  - rectangle{}
    - x* [real_vec]
    - y* [real_vec]
  - cuboid{}
    - x* [real_vec]
    - y* [real_vec]
    - z* [real_vec]
  - …
  - contact{}
    - name [string]
    - remove{}
  - binary{}
    - name* [string]
  - ternary_constant{}
    - name* [string]
    - alloy_x* [real]
  - …
  - quaternary_constant{}
    - name* [string]
    - alloy_x* [real]
    - alloy_y* [real]
  - …
  - quinternary_constant{}
    - name* [string]
    - alloy_x* [real]
    - alloy_y* [real]
    - alloy_z* [real]
  - …
  - doping{}
    - remove{}
    - constant{}
      - name* [string]
      - conc* [real]
      - add [yes, no]
    - …
  - generation{}
    - remove{}
    - constant{}
      - rate* [real]
      - constant [yes, no]
    - …
  - injection{}
    - remove{}
    - constant{}
      - rate* [real]
      - add [yes, no]
    - …
  - integrate{}
    - label [string]
    - electron_density{}
    - hole_density{}
    - piezo_density{}
    - pyro_density{}
    - polarization_density{}

strain{}

- debuglevel [int]
- pseudomorphic_strain{}
- minimized_strain{}
- piezo_density [yes, no]
- pyro_density [yes, no]
- second_order_piezo [yes, no]
- growth_direction [int_vec]
- linear_solver{}
  - iterations [int]
  - abs_accuracy [real]
  - rel_accuracy [real]
  - use_cscg [yes, no]
  - force_diagonal_preconditioner [yes, no]
- import_strain{}
  - import_strain* [string]
  - coordinate_system [crystal, simulation]
- output_hydrostatic_strain{}, output_elastic_energy_density{}, output_lattice_constants{}, output_elastic_constants{}, output_piezo_constants{}, output_second_order_piezo_constants{}, output_pyro_constants{}
  - boxes [yes, no]
- output_strain_tensor{}, output_distortion_tensor{}, output_stress_tensor{}, output_polarization_vector{}
  - crystal_system [yes, no]
  - simulation_system [yes, no]
  - boxes [yes, no]
- output_displacement{}, output_force_density{}
  - crystal_system [yes, no]
  - simulation_system [yes, no]
- output_polarization_charges{}

currents{}

- mobility_model [constant, masetti, arora, minimos]
- high_field_saturation{}
  - alpha_electrons* [real]
  - beta_electrons* [real]
  - vsat_electrons* [real]
  - alpha_holes* [real]
  - beta_holes* [real]
  - vsat_holes* [real]
- recombination_model{}*
  - SRH [yes, no]
  - Auger [yes, no]
  - radiative [yes, no]
  - enable_generation [yes, no]
- debuglevel [int]
- linear_solver{}
  - iterations [int]
  - abs_accuracy [real]
  - rel_accuracy [real]
  - dkr_value [real]
  - use_cscg [yes, no]
  - force_diagonal_preconditioner [yes, no]
  - force_iteration [yes, no]
  - extended_accuracy [int]
- insulator_bandgap [real]
- minimum_density[real]
- minimum_density_factor [real_vec]
- maximum_density [real]
- maximum_density_factor [real_vec]
- minimal_recombination [yes, no]
- output_fermi_levels{}
- output_fermi_level_difference{}
- output_velocities{}
- output_currents{}
- output_power_density{}
- output_mobilities{}
  - boxes [yes, no]
- output_recombination{}
- output_injection{}

cbr{}

- name* [string]
- lead{}
  - name* [string]
- rel_min_energy [real]
- rel_max_energy [real]
- abs_min_energy [real]
- abs_max_energy [real]
- delta_energy [real]
- ildos [yes, no]
- options [real_vec]

contacts{}

- vacuum_level
- fermi_electron{}, fermi_hole{}, fermi{}, zero_field{}, charge_neutral{}
  - name* [string]
  - bias* [real_vec]
  - steps [int]
- schottky{}
  - name* [string]
  - bias* [real_vec]
  - steps [int]
  - barrier [real]
  - work_function [real]
- ohmic{}
  - name* [string]
  - bias* [real_vec]
  - steps [int]
  - shift [real]
- long_directory_names [yes, no]

impurities{}

- donor{}, acceptor{}
  - name* [string]
  - degeneracy* [int]
  - energy* [real]
- charge{}
  - name* [string]
  - type* [positive, negative]

run{}

- structure_only{}
  - last_region [int]
- strain{}
- solve_strain{}
- poisson{}
- solve_poisson{}
- current_poisson{}, solve_current_poisson{}
  - fermi_limit [real]
  - multi_stage_solve [yes, no]
  - fast_poisson [yes, no]
  - use_newmethod [yes, no]
  - system_solve [yes, no]
  - iterations [int]
  - current_repetitions [int]
  - limit_repetitions [yes, no]
  - residual [real]
  - residual_fermi [real]
  - alpha_fermi [real]
  - alpha_iterations [int]
  - alpha_scale [real]
  - output_log [yes, no]
- outer_iteration{}
  - residual [real]
  - iterations [int]
  - use_subspace [yes, no]
  - subspace_iterations [int]
  - subspace_residual_factor [real]
  - fixed_fermi_levels [yes, no]
  - fermi_limit [real]
  - current_repetitions [int]
  - limit_repetitions [yes, no]
  - residual_fermi [real]
  - alpha_fermi [real]
  - alpha_iterations [int]
  - alpha_scale [real]
  - alpha_potential [real]
  - output_log [yes, no]
- quantum{}
- solve_quantum{}
- quantum_density{}
  - residual [real]
  - iterations [int]
  - use_subspace [yes, no]
  - subspace_iterations [int]
  - subspace_residual_factor [real]
  - output_log [yes, no]
- quantum_poisson{}
  - residual [real]
  - iterations [int]
  - use_subspace [yes, no]
  - subspace_iterations [int]
  - subspace_residual_factor [real]
  - alpha_potential [real]
  - output_log [yes, no]
- quantum_current_poisson{}
  - residual [real]
  - iterations [int]
  - use_subspace [yes, no]
  - subspace_iterations [int]
  - subspace_residual_factor [real]
  - fermi_limit [real]
  - current_repetitions [int]
  - limit_repetitions [yes, no]
  - residual_fermi [real]
  - alpha_fermi [real]
  - alpha_iterations [int]
  - alpha_scale [real]
  - alpha_potential [real]
  - output_log [yes, no]
- optics{}

classical{}*

- Gamma{}, X{}, Delta{}, L{},HH{}, LH{}, SO{}
  - output_bandedge{}
    - averaged [yes, no]
- carrier_statistics [maxwell_boltzmann, fermi_dirac]
- energy_distribution{}, energy_resolved_density{}
  - min* [real]
  - max* [real]
  - energy_resolution [real]
  - only_quantum_regions [yes, no]
- emission_spectrum{}
  - refractive_index [real]
  - output_spectra{}*
    - emission [yes, no]
    - gain [yes, no]
    - absorption [yes, no]
    - stimulated_emission [yes, no]
    - spectra_over_energy [yes, no]
    - spectra_over_wavelength [yes, no]
    - spectra_over_frequency [yes, no]
    - spectra_over_wavenumber [yes, no]
    - photon_spectra [yes, no]
    - power_spectra [yes, no]
  - output_photon_density [yes, no]
  - output_power_density [yes, no]
- irradiation{}
  - min_wavelength [real]
  - max_wavelength [real]
  - min_energy [real]
  - max_energy [real]
  - energy_resolution* [real]
  - illumination{}*
    - direction_x [int]
    - direction_y [int]
    - direction_z [int]
    - database_spectrum{}
      - name* [string]
      - concentration [real]
    - import_spectrum{}
      - import_from* [string]
      - cutoff* [yes, no]
      - absolute_intensities [yes, no]
      - concentration [real]
    - constant_spectrum{}
      - irradiance*
    - planck_spectrum{}
      - irradiance* [real]
      - temperature* [real]
    - lorentzian_spectrum{}, gaussian_spectrum{}
      - irradiance* [real]
      - wavelength [real]
      - energy [real]
      - width [real]
      - gamma [real]
  - reflectivity{}
    - database_spectrum{}
      - name* [string]
    - import_spectrum{}
      - import_from* [string]
      - cutoff* [yes, no]
    - constant_spectrum{}
      - reflectivity* [real]
  - absorption{}
    - database_spectrum{}
      - name* [string]
    - import_spectrum{}
      - import_from* [string]
      - cutoff* [yes, no]
    - constant_spectrum{}
      - absorption* [real]
  - output_spectra{}*
    - illumination [yes, no]
    - reflectivity [yes, no]
    - absorption [yes, no]
    - spectra_over_energy [yes, no]
    - spectra_over_wavelength [yes, no]
    - spectra_over_frequency [yes, no]
    - spectra_over_wavenumber [yes, no]
  - output_light_field [yes, no]
  - photo_generation{}
    - output [yes, no]
    - output_spectrum [yes, no]
    - output_energy_resolved [yes, no]
    - output_quantum_efficiency [yes, no]
- output_bandgap{}
  - averaged [yes, no]
- output_bandedges{}
  - profiles [Gamma, X, Delta, L, HH, LH, SO, electron_fermi_level hole_fermi_level]
  - averaged [yes, no]
- output_carrier_densities{}
- output_ionized_dopant_densities{}
- output_energy_resolved_densities{}
- output_intrinsic_density{}
  - boxes [yes, no]

poisson{}

- debuglevel [int]
- charge_neutral [yes, no]
- import_potential{}
  - import_from* [string]
  - component_number [int]
- reference_potential [real]
- electric_field{}
  - direction [real_vec]
  - strength [real]
- newton_solver{}
  - iterations [int]
  - search_steps [int]
  - residual [real]
  - gradient_shift [real]
- linear_solver{}
  - iterations [int]
  - abs_accuracy [real]
  - rel_accuracy [real]
  - dkr_value [real]
  - use_cscg [yes, no]
  - force_diagonal_preconditioner [yes, no]
  - force_iteration [yes, no]
- bisection{}
  - delta [real]
  - residual [real]
  - iterations [int]
- output_potential{}
- output_electric_field{}
- output_electric_displacement{}
- output_electric_polarization{}
- output_dielectric_tensor{}
- boxes [yes, no]

optics{}

- debuglevel [int]
- region{}
  - name* [string]
  - energy_allowed_only [yes, no]
  - make_spin_degenerate [yes, no]
  - spin_align [yes, no]
  - interband [yes, no]
  - intraband [yes, no]
  - interband_approximation [yes, no]
  - intraband_approximation [yes, no]
  - energy_threshold [real]
  - transition_threshold [real]
  - occupation_threshold [real]
  - occupation_ignore [yes, no]
  - occupation_interpolate_invfermi [yes, no]
  - occupation_const_fermilevel [yes, no]
  - spontaneous_emission [yes, no]
  - output_energies [yes, no]
  - output_occupations [yes, no]
  - output_transitions [yes, no]
  - output_spinor_components [yes, no]
  - output_spectra{}*
    - output_components [yes, no]
    - spectra_over_energy [yes, no]
    - spectra_over_wavelength [yes, no]
    - spectra_over_frequency [yes, no]
    - spectra_over_wavenumber [yes, no]
  - polarization{}*
    - name* [string]
    - re [real_vec]
    - im [real_vec]
  - refractive_index [real]
  - normalization_volume [real]
  - energy_resolution [real]
  - energy_max [real]
  - energy_min [real]
  - energy_broadening_gaussian [real]
  - energy_broadening_lorentzian [real]
  - kramers_kronig{}
    - im_epsilon_extension [real]
    - im_epsilon_rescale [real]
    - delta_static_epsilon [real]
    - delta_position [real]
    - use_for_absorption [yes, no]
  - k_integration{}
    - relative_size [real]
    - symmetry [int]
    - num_points [int]
    - num_subpoints [int]
    - num_totalsubpoints [int]
    - force_k0_subspace [yes, no]
  - symmetrize_operators [yes, no]
  - central_differences [yes, no]

quantum{}

- debuglevel [int]
- allow_overlapping_regions [yes, no]
- exchange_correlation{}
  - type [lda, lsda]
  - initial_spin_pol [real]
  - output_spin_polarization {}
  - output_exchange_correlation{}
- region{}
  - name* [string]
  - no_density [yes, no]
  - quantize_x{}
  - quantize_y{}
  - quantize_z{}
  - x* [real_vec]
  - y [real_vec]
  - z [real_vec]
  - array_x{}, array_y{}, array_z{}, array2_x{}, array2_y{}, array2_z{}
    - shift* [real]
    - min [int]
    - max* [int]
  - boundary{}
    - x [dirichlet, neumann, cbr]
    - y [dirichlet, neumann, cbr]
    - z [dirichlet, neumann, cbr]
    - classical_boundary_x [yes, no]
    - classical_boundary_y [yes, no]
    - classical_boundary_z [yes, no]
    - num_classical_x [int_vec]
    - num_classical_y [int_vec]
    - num_classical_z [int_vec]
  - Gamma{}, X{}, Delta{}, L{}, HH{}, LH{}, SO{}
    - accuracy [real]
    - iterations [int]
    - k_integration{}
      - relative_size [real]
      - max_symmetry [no, C2, full]
      - num_points [int]
      - num_subpoints [int]
      - force_k0_subspace [yes, no]
    - dispersion{}
      - full{}
        - name* [string]
        - kxgrid{}, kygrid{}, kzgrid{}
          - line{}*
            - pos* [real]
            - spacing* [real]
      - path{}
        - name* [string]
        - point{}*
          - k* [real_vec]
        - spacing [real]
        - num_points [int]
      - lines{}
        - name* [string]
        - k_max* [real]
        - spacing [real]
      - superlattice{}
        - name* [string]
        - num_points [int]
        - num_points_x [int]
        - num_points_y [int]
        - num_points_z [int]
      - output_dispersions{}
        - max_num [int]
      - output_masses{}
        - max_num [int]
    - num_ev* [int]
    - lapack{}
    - arpack{}
    - preconditioner [polynomial, chebyshev, legendre]
    - order_polynomial [int]
    - order_chebyshev [int]
    - order_legendre [int]
    - cutoff [real]
    - abs_cutoff [real]
    - force_complex_solver [yes, no]
  - kp_6band{}
    - accuracy [real]
    - iterations [int]
    - k_integration{}
      - relative_size [real]
      - max_symmetry [no, C2, full]
      - num_points [int]
      - num_subpoints [int]
      - force_k0_subspace [yes, no]
    - dispersion{}
      - full{}
        - name* [string]
        - kxgrid{}, kygrid{}, kzgrid{}
          - line{}*
            - pos* [real]
            - spacing* [real]
      - path{}
        - name* [string]
        - point{}*
          - k* [real_vec]
        - spacing [real]
        - num_points [int]
      - lines{}
        - name* [string]
        - k_max* [real]
        - spacing [real]
      - superlattice{}
        - name* [string]
        - num_points [int]
        - num_points_x [int]
        - num_points_y [int]
        - num_points_z [int]
      - output_dispersions{}
        - max_num [int]
      - output_masses{}
        - max_num [int]
    - num_ev* [int]
    - lapack{}
    - arpack{}
    - preconditioner [polynomial, chebyshev, legendre]
    - order_polynomial [int]
    - order_chebyshev [int]
    - order_legendre [int]
    - cutoff [real]
    - abs_cutoff [real]
    - kp_parameters{}
      - use_Luttinger_parameters [yes, no]
      - approximate_kappa [yes, no]
  - kp_8band{}
    - accuracy [real]
    - iterations [int]
    - k_integration{}
      - relative_size [real]
      - max_symmetry [no, C2, full]
      - num_points [int]
      - num_subpoints [int]
      - force_k0_subspace [yes, no]
    - dispersion{}
      - full{}
        - name* [string]
        - kxgrid{}, kygrid{}, kzgrid{}
          - line{}*
            - pos* [real]
            - spacing* [real]
      - path{}
        - name* [string]
        - point{}*
          - k* [real_vec]
        - spacing [real]
        - num_points [int]
      - lines{}
        - name* [string]
        - k_max* [real]
        - spacing [real]
      - superlattice{}
        - name* [string]
        - num_points [int]
        - num_points_x [int]
        - num_points_y [int]
        - num_points_z [int]
      - output_dispersions{}
        - max_num [int]
      - output_masses{}
        - max_num [int]
    - lapack{}
    - arpack_inv{}
    - num_electrons [int]
    - num_holes [int]
    - shift [real]
    - abs_shift [real]
    - shift_window [int]
    - shift_min_CB [real]
    - shift_max_VB [real]
    - tunnelling [yes, no]
    - classify_kspace [int]
    - threshold_classification [real]
    - full_band_density [yes, no]
    - linear_solver{}
      - iterations [int]
      - abs_accuracy [real]

- rel_accuracy [real]
- use_cscg [yes, no]
- force_diagonal_preconditioner [yes, no]

- spurious_handling [real_vec]
- kp_parameters{}
  - use_Luttinger_parameters [yes, no]
  - from_6band_parameters [yes, no]
  - evaluate_S [yes, no]
  - rescale_S_to [real_vec]
  - approximate_kappa [yes, no]

- intraband_matrix_elements{}, dipole_moment_matrix_elements{}
  - Gamma{}, X{}, Delta{}, L{}, HH{}, LH{}, SO{}, KP6{}, KP8{}
    - direction [real_vec]
  - output_matrix_elements [yes, no]
  - output_transition_energies [yes, no]
  - output_oscillator_strengths [yes, no]
- interband_matrix_elements{}
  - Gamma{}, X{}, Delta{}, L{}, HH{}, LH{}, SO{}, KP6{}, KP8{}
  - output_matrix_elements [yes, no]
  - output_transition_energies [yes, no]
- transition_energies{}
  - HH_Gamma{}
  - LH_Gamma{}
  - SO_Gamma{}
  - KP6_Gamma{}
  - HH_X{}
  - LH_X{}
  - SO_X{}
  - HH_Delta{}
  - LH_Delta{}
  - SO_Delta{}
  - HH_L{}
  - LH_L{}
  - SO_L{}
  - Gamma{}
  - X{}
  - Delta{}
  - L{}
  - HH{}
  - LH{}
  - SO{}
  - KP6{}
  - KP8{}
- calculate_lifetime{}
  - phonon_energy [real]
- bulk_dispersion{}
  - full{}
    - name* [string]
    - position{}*
      - x* [real]
      - y [real]
      - z [real]
    - shift_holes_to_zero [yes, no]
    - kxgrid{}*, kygrid{}*, kzgrid{}*
      - line{}*
        - pos* [real]
        - spacing* [real]
  - path{}
    - name* [string]
    - position{}*
      - x* [real]
      - y [real]
      - z [real]
    - shift_holes_to_zero [yes, no]
    - point{}*
      - k* [real_vec]
    - spacing* [real]
    - num_points [int]
  - lines{}
    - name* [string]
    - position{}*
      - x* [real]
      - y [real]
      - z [real]
    - shift_holes_to_zero [yes, no]
    - k_max* [real]
    - spacing* [real]
  - output_bulk_dispersions{}
  - output_masses{}
- output_wavefunctions{}
  - max_num [int]
  - all_k_points [yes, no]
  - amplitudes [yes, no, S_X_Y_Z, CB_HH_LH_SO]
  - probabilities [yes, no, S_X_Y_Z, CB_HH_LH_SO]
  - in_one_file [yes, no]
  - scale [real]
  - structured [yes, no]
  - energy_shift [shifted, not_shifted, both]
  - include_eigenvalues_in_shifted_files [yes, no]
- output_subband_densities{}
  - max_num [int]
  - in_one_file [yes, no]
- output_quantum_densities{}
- output_rotated_inverse_mass_tensor{}
  - boxes [yes, no]
  - structured [yes, no]

import{}

- ...

database{}

- ...

output{}

- ...