

- Fig.2.2

TB data: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK

MLWF data: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier

- Fig.2.4 https://nanohub.org/tools/nemo/svn/trunk/NEMO/regression_test/numerical_tests/readin_wannier/gated_sch_poisson

- slides:

2016 sispad Poster: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/Documentation/sispad2016_poster_v4.pptx

2017 IWCN slides: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/Documentation/IWCN_2017_james_v1.pptx

- Bandstructure inputs / Wannier parameters for 2D materials.

- a. MoS2:

bulk: https://nanohub.org/tools/nemo/svn/trunk/NEMO/regression_test/numerical_tests/readin_wannier/Bandstructure_SO_MoS2_1layer

layer dependant: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK/input

- b. MoSe2 :

bulk: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/All_material_gathering/MoSe2/MoSe2_wannier_bulk.in

layer dependant: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/MoSe2/input

- c. MoTe2: bulk: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/All_material_gathering/MoTe2_smaller/5NEM05_pseudo_kfix/MoTe2_wannier_bulk.in
- d. WS2 https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/All_material_gathering/WS2_kuang/5NEM05_pseudo/WS2_wannier_bulk.in
- e. WSe2 https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/All_material_gathering/WSe2/5NEM05_pseudo/WSe2_wannier_bulk.in
- f. BP bulk https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/All_material_gathering/BP_bulk/4_nemo/bulk.in
- Fig.3.2 https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/bulk_multisize/transform
- Fig.3.3
Figure: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/EK_compare_wannier_dft/EK2_energies5_3.datEKcombo.png
MLWF input : https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier/input
DFT input :
1layer: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/1layer_daniel/
5layer: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_dft/smaller_GGA/5layer_yao

- Fig.3.4

regression test : Figure: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/Ec_two_valleys_diff.png https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/Ev_two_valleys_diff.png Script for replotting : https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/plot.sh

- Fig.3.5 Figure: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/Ec_two_valleys_diff.png https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/Ev_two_valleys_diff.png Script for replotting : https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/plot.sh

- Fig.3.6

(a) https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/eff_mc_Q.png

raw data:

[../step6_EK_wannierS0/EK/mc_left_of_point2.temp](#)

[MoSe2/EK/mc_mid_of_point2.temp](#)

[WS2/EK/mc_mid_of_point2.temp](#)

[MoTe2/EK/mc_mid_of_point2.temp](#)

[WSe2/EK/mc_mid_of_point2.temp](#)

(b) https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/eff_mc_

K.png

raw data:

../step6_EK_wannierS0/EK/mc_left_of_point3.temp

MoSe2/EK/mc_mid_of_point3.temp

WS2/EK/mc_mid_of_point3.temp

MoTe2/EK/mc_mid_of_point3.temp

WSe2/EK/mc_mid_of_point3.temp

(c) https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/eff_mv_

G.png

raw data: ../step6_EK_wannierS0/EK/mv_right_of_point1.temp

MoSe2/EK/mv_mid_of_point1.temp

WS2/EK/mv_mid_of_point1.temp

MoTe2/EK/mv_mid_of_point1.temp

WSe2/EK/mv_mid_of_point1.temp

(d) https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier_All/eff_mv_

K.png raw data:

../step6_EK_wannierS0/EK/mv_left_of_point3.temp

MoSe2/EK/mv_mid_of_point3.temp

WS2/EK/mv_mid_of_point3.temp

- Fig.3.7

https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step5_DOS_with_cart_wannier/DOS/

Figure: ./DOS_layer_shift.png

Raw data: ./1_layer__ ./2_layer__ ./3_layer__ ./4_layer__ inputs: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step5_DOS_with_cart_wannier/input

- Fig.3.8 https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step1_non_delta_macro_wannier_all_TMDs/
figure: EcEfdopingplot.png
input folder for each material is listed
- Fig.3.9
input: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step6_EK_wannier/bulk/bulk_primitive2_3.in
- Fig.3.10, Fig.3.11
regression test : https://nanohub.org/tools/nemo/svn/trunk/NEMO/regression_test/numerical_tests/readin_wannier/bulk_gated_wavefunction https://nanohub.org/tools/nemo/svn/trunk/NEMO/regression_test/numerical_tests/readin_wannier/gated_sch_poisson
- Fig.3.12 https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step3_300nm_All_TMDs/MoS2_Wannier_S0_epsilon_doping_larger2e19_radius_realistic1.26
- Fig.3.13
figures: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step3_300nm_All_TMDs/MoS2_Wannier_S0_epsilon_doping_larger2e19_radius_realistic/run_layer_5_Vg_0_Nd_1_pri_wannier_S0/EK2_energies.datEKcombo.png
Raw Data:
https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/step3_300nm_All_TMDs/MoS2_Wannier_S0_epsilon_doping_larger2e19_radius_realistic/run_layer_5_Vg_0_Nd_1_pri_wannier_S0
<https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/>

sphinx_log/source/201411/MoS2_YuHe/N_Pot/step3_300nm_All_TMDs/MoS2_Wannier_SO_epsilon_doping_larger2e19_radius_realistic/run_layer_5_Vg_100_Nd_1_pri_wannier_SO

- Fig.3.14

Data: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/PL/voltage_61

- Fig.3.15

Data: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201411/MoS2_YuHe/N_Pot/PL_comparison/NEMO5_Band_extraction_E.xlsx

- Presentation/Reports:

2019 IWCN: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/Documentation/IWCN2019.pptx

2018 NUSOD: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/Documentation/2018nusod.pptx

2018 SISPAD: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/Documentation/2018sispad_slide.pptx

- Fig.5.1

Folder: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/4_flat_band_mobility

figure: eta_mobility.png

raw data for the plot :

eta_mobility_1e20input_refine_bandedge_uniform_fixedK_flat_contacteta.

in

eta_mobility_1e20input_refine_bandedge_uniform_fixedK_hole_flat_contacteta.

in

inputs templates(requires the script to change parameters):

```
input_refine_bandedge_uniform_fixedK_hole_flat_contacteta.in
```

```
input_refine_bandedge_uniform_fixedK_flat_contacteta.in
```

Script to produce all input decks ramping different parameters e.g. voltages doping:

```
./submit_voltage.sh sub 0 1e20 input_refine_bandedge_uniform_fixedK_flat_contacteta.in
```

```
./submit_voltage.sh sub 0 1e20 input_refine_bandedge_uniform_fixedK_hole_flat_contacteta.in
```

- Fig. 5.3

DD raw data folder:

```
https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_updatedparam_update_mobi/well_Vd3.000000e+00_doping1e20pn1.in_jac_9_emesh_32_kmesh_20_kmax_0.5
```

DD input: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_updatedparam_update_mobi/pn1.in

NEGF raw data folder:

```
https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta/Vd3.000000e+00_doping1e20input_refine_bandedge_uniform_fixedK_etaleads_urback.in_jac_9_emesh_128_kmesh_40_kmax_0.1_oneshot
```

Contour raw data:

```
bprgf_e_backward_solver_device_energy_resolved_k_integrated_density.dat
```

```
bprgf_h_backward_solver_device_energy_resolved_k_integrated_density.dat
```

spatial density data: debug_n.dat debug_p.dat

input deck :

```
https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/
sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_
semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta/Vd3.000000e+00_
doping1e20input_refine_bandedge_uniform_fixedK_etaleads_urbac.in_jac_
9_emesh_128_kmesh_40_kmax_0.1_oneshot_/temp_3.000000e+00_1e20input_
refine_bandedge_uniform_fixedK_etaleads_urbac.in_jac_9_emesh_128_kmesh_
40_kmax_0.1.in
```

- Fig. 5.4

DD data for 3.0V: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_updatedparam_update_mobi/well_Vd3.000000e+00_doping1e20pn1.in_jac_9_emesh_32_kmesh_20_kmax_0.5

DD data for 3.6V https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_updatedparam_update_mobi/well_Vd3.600000e+00_doping1e20pn1.in_jac_9_emesh_32_kmesh_20_kmax_0.5

Band profile: Ec.dat Ev.dat

spatially resolved recombination: A.dat B.dat C.dat

NEGF data for 3.0V:

```
input https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/
sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_
semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta/temp_3.000000e+
00_1e20input_refine_bandedge_uniform_fixedK_etaleads_urbac.in_jac_
9_emesh_128_kmesh_40_kmax_0.1.in
```

folder https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta/Vd3.000000e+00_

doping1e20input_refine_bandedge_uniform_fixedK_etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_0.1trial_0

NEGF data for 3.6V:

input https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta/Vd3.600000e+00_doping1e20input_refine_bandedge_uniform_fixedK_etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_0.1trial_0
 folder https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta/temp_3.600000e+00_1e20input_refine_bandedge_uniform_fixedK_etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_0.1.in

- Fig. 5.5

DD Folder: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_updatedparam_update_mobi/ DD IV raw data: IVtotal_1e20pn1.

in total_re

NEGF data folder: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta

NEGF IV data: wellIVtotal_1e20input_refine_bandedge_uniform_fixedK_well_etaleads.in wellIVrecomb_1e20input_refine_bandedge_uniform_fixedK_well_etaleads.in

NEGF job script: ./overlord.sh

Simulation Results:

poisson calculation output: Vd*_doping1e20input_refine_bandedge_uniform_fixedK_well_etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_0.1trial_0

0

current conservation loop output : Vd*_doping1e20input_refine_bandedge_
uniform_fixedK_well_etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_
0.1_oneshot_

- Fig.5.6

DD data Folder: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_well_capture_escape_with_radiative_SRH_Auger_for_bound_states_with_pn_update_mobi/well_Vd2.600000e+00_doping1e20optimizeEkmesh_jac_9_emesh_32_kmesh_20_kmax_0.5

Figure: np_xnm_log2.png Ec.png Ev.png

input: ../qw1.in

NEGF data Folder: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta/Vd2.600000e+00_doping1e20input_refine_bandedge_uniform_fixedK_well_etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_0.1_oneshot_

input: temp_2.600000e+00_1e20input_refine_bandedge_uniform_fixedK_well_etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_0.1.in

Contour raw data:

bprgf_e_backward_solver_device_energy_resolved_k_integrated_dos.dat

bprgf_h_backward_solver_device_energy_resolved_k_integrated_dos.dat

density data: debug_n.dat debug_p.dat

- Fig.5.7

DD File :

https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_well_capture_escape_with_radiative_SRH_Auger_for_bound_states_with_pn_update_mobi/well_Vd4.000000e+00_doping1e20optimizeEkmesh_jac_9_emesh_

32_kmesh_20_kmax_0.5

Band profile: Ec.dat Ev.dat

NEGF File:

folder: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta/Vd4.000000e+00_doping1e20input_refine_bandedge_uniform_fixedK_well_etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_0.1_one-shot_

contour data:

bprgf_e_backward_solver_device_energy_resolved_k_integrated_density.

dat

bprgf_h_backward_solver_device_energy_resolved_k_integrated_density.

dat

- Fig. 5.8

Figure file:

https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_well_capture_escape_with_radiative_SRH_Auger_for_bound_states_with_pn_update_mobi/IVlog_eta0.05_comp.png

https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_well_capture_escape_with_radiative_SRH_Auger_for_bound_states_with_pn_update_mobi/IV_eta0.05_comp.png

NEGF data folder:

https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_contacteta

processing commands is in ./overlord.sh

IV raw data :

wellIVtotal_1e20input_refine_bandedge_uniform_fixedK_well_etaleads.

in

wellIVrecomb_1e20input_refine_bandedge_uniform_fixedK_well_etaleads.

in

raw data files: Vd*_doping1e20input_refine_bandedge_uniform_fixedK_well_

etaleads_urbach.in_jac_9_emesh_128_kmesh_40_kmax_0.1_oneshot_Vd*_doping1e20in

refine_bandedge_uniform_fixedK_well_etaleads_urbach.in_jac_9_emesh_

128_kmesh_40_kmax_0.1trial_0

DD data folder:

https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_well_capture_escape_with_radiative_SRH_Auger_for_bound_states_with_pn_update_mobi/

- Fig. 5.9

NEGF folder :

https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_EcEv_sym_exp_withpoisson_solar_contacteta

input template:

input_refine_bandedge_uniform_fixedK_well_contacteta_100k.in

input_refine_bandedge_uniform_fixedK_well_contacteta.in

script: overlord.sh

figure: IVnew350k_100knew.png

raw data: IV_350KIVsolar_half_350kIVsolar_350kIVsolar_100k, well_new_

IVtotal_1e20input_refine_bandedge_uniform_fixedK_well_contacteta.in_

gen0, well_new_IVtotal_1e20input_refine_bandedge_uniform_fixedK_well_

contacteta.in_gen1.325E-18, well_new_IVtotal_1e20input_refine_bandedge_

uniform_fixedK_well_contacteta.in_gen2.65E-18,well_new_IVtotal_1e20input_refine_bandedge_uniform_fixedK_well_contacteta_100k.in_gen2.65E-18

DD folder : https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/silvaco_DD_comparison/pn_junction_well_capture_escape_with_radiative_SRH_Auger_for_bound_states_with_pn_update_mobi_solarcell/photogeneration_after_fix/

input decks: well_temp_2.600000e+00_1e20optimizeEkmesh_jac_9_emesh_32_kmesh_20_kmax_0.5_m.in,well_temp_2.600000e+00_1e20optimizeEkmesh_jac_9_emesh_32_kmesh_20_kmax_0.5_m_solar.5.in,well_temp_2.600000e+00_1e20optimizeEkmesh_jac_9_emesh_32_kmesh_20_kmax_0.5_m_solar.in,well_temp_2.600000e+00_1e20optimizeEkmesh_jac_9_emesh_32_kmesh_20_kmax_0.5_m_solar_100k.in

- Fig. 5.11 and Fig. 5.10 :

https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201711_buttikerprobe/3_e_h_coupled_resonance_expdecay_semiclassical_GaN_20bandTB_sym_exp_withpoisson_contacteta/

input: input_refine_bandedge_uniform_fixedK_well_etaleads_urbach_20bands.in

script: ./overlord.sh

raw data for each bias is stored in Vd*_doping1e20input_refine_bandedge_uniform_fixedK_well_etaleads_urbach_20bands.in_jac_9_emesh_128_kmesh_40_kmax_0.1_oneshot_/_

- mobility calculation:

raw data: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/DanielValencia/MoS2_BP/transport_poisson

script:

input : BP_homo_sancho_x.in MoS2_homo_sancho_x.in

- Fig. 6.2 MLWF data resides in : https://nanohub.org/groups/klimeck/svn/trunk/StudentData/DanielValencia/MoS2_BP/NEMO5_readin_new_param_vasp

(a)EK_BP2_energies.datEKcombo.png (b)EK_MoS2_energies.datEKcombo.png

(c)EK_all_energies.datEKcombo.png

command and input within the folder:

```
mpirun -np 24 NEMO5_brown3 BP_MoS2_readin.in
```

```
mpirun -np 24 NEMO5_brown3 MoS2_readin.in
```

```
mpirun -np 24 NEMO5_brown3 BP_readin.in
```

DFT data:

BP with MoS2 https://nanohub.org/groups/klimeck/svn/trunk/StudentData/DanielValencia/MoS2_BP/BP_MoS2_dft_vaspwa_final

BP : https://nanohub.org/groups/klimeck/svn/trunk/StudentData/DanielValencia/MoS2_BP/BP_1layer_dft

MoS2 : https://nanohub.org/groups/klimeck/svn/trunk/StudentData/DanielValencia/MoS2_BP/MoS2_1layer_dft

- Fig. 6.5

exp data : https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201709_BPMoS2/exp_data

script: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201709_BPMoS2/IV_AAP/submit_vbo_vbg.sh

- Fig. 6.6

(a) different length

14nm overlap: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201709_BPMoS2/IV_AAP/submit_long_overlap.sh

6nm overlap: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201709_BPMoS2/IV_AAP/submit_shortoverlap.sh

(b) different rates script: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201709_BPMoS2/IV_AAP/submit_vbo_rates.sh

(c) different vbo: https://nanohub.org/groups/klimeck/svn/trunk/StudentData/kuangchungwang/sphinx_log/source/201709_BPMoS2/IV_AAP/submit_vbo.sh

Script Usage:

Poisson self-consistent calculation: `./submit_*.sh sub sub`

current conservation calculation: `./submit_*.sh sub seq_freezeV`