Synopsys® Silicon to Software™

Accurate atomistic simulations of solar-cell devices including temperature effects

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Ulrik Vej-Hansen, PhD, Application Engineer, Synopsys QuantumATK team

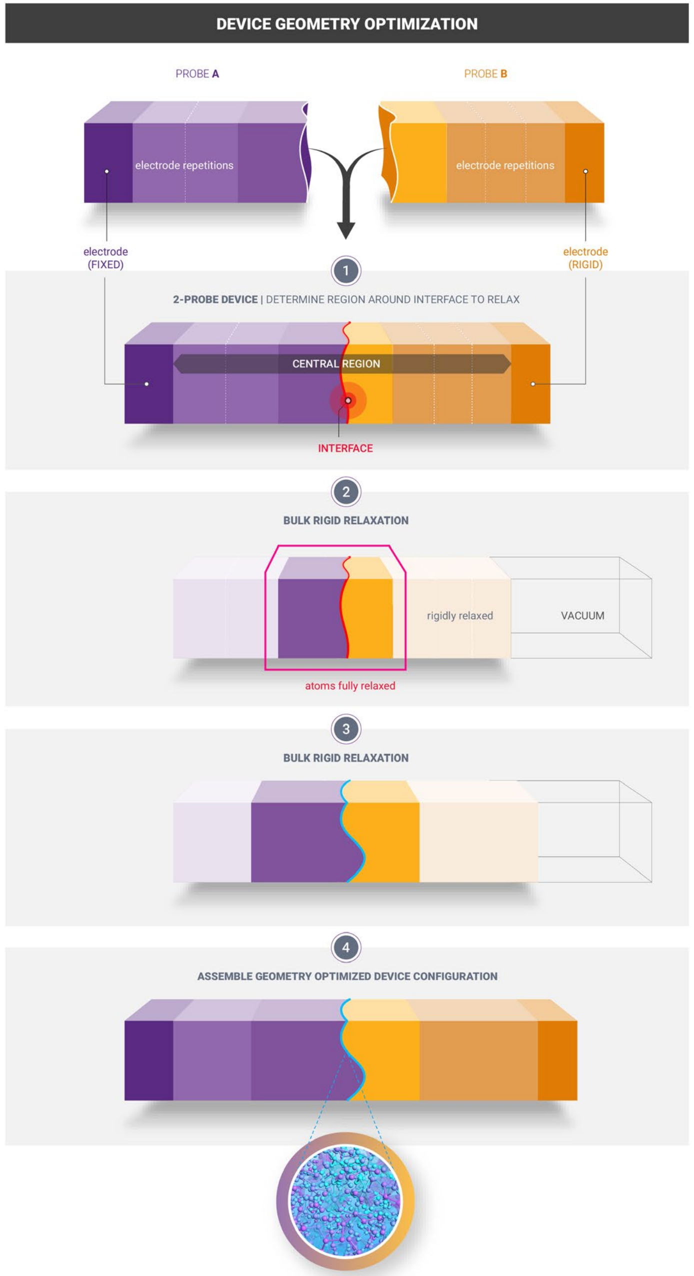
Meet us at

IEDM, 64th International Electron Devices Meeting
Dec 1-5, 2018
San Francisco, US

Arrange a meeting/demo with us:
quantumatk@synopsys.com

One more webinar in 2018

Register on www.quantumwise.com



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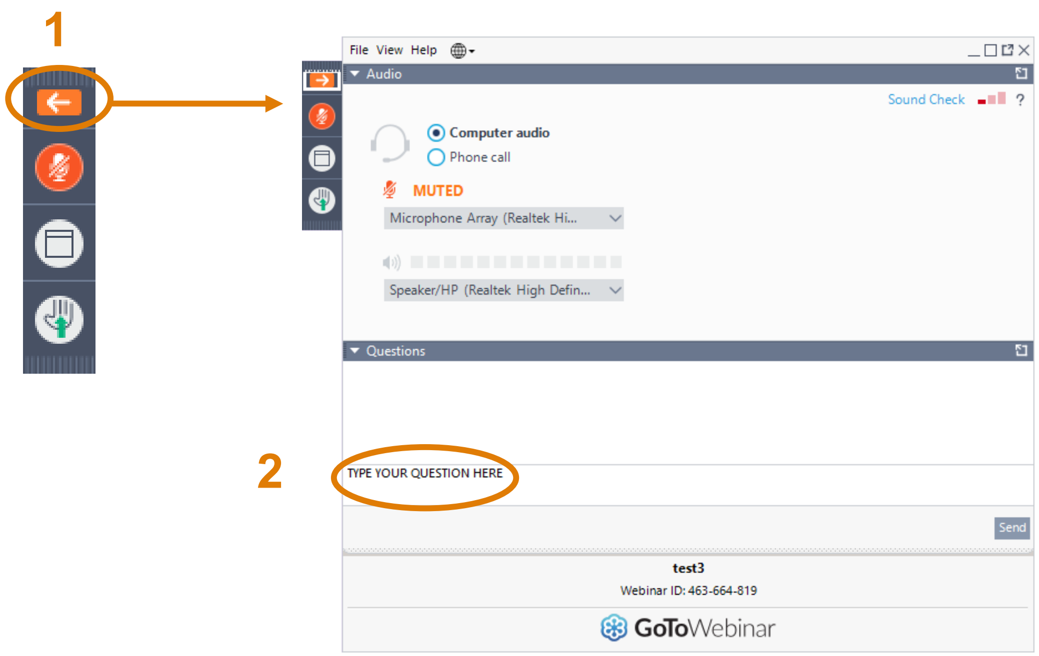
How to ask questions?

You can click on (Windows, macOS) or on (Linux) (1). A new window will open in which you can type your question (2). You can write questions during the webinar, that will be addressed during the Q&A session at the end of the webinar or after the webinar is concluded.

Windows/Mac



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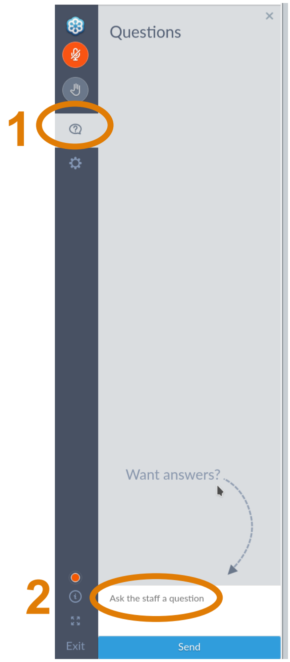


Outline

Motivation

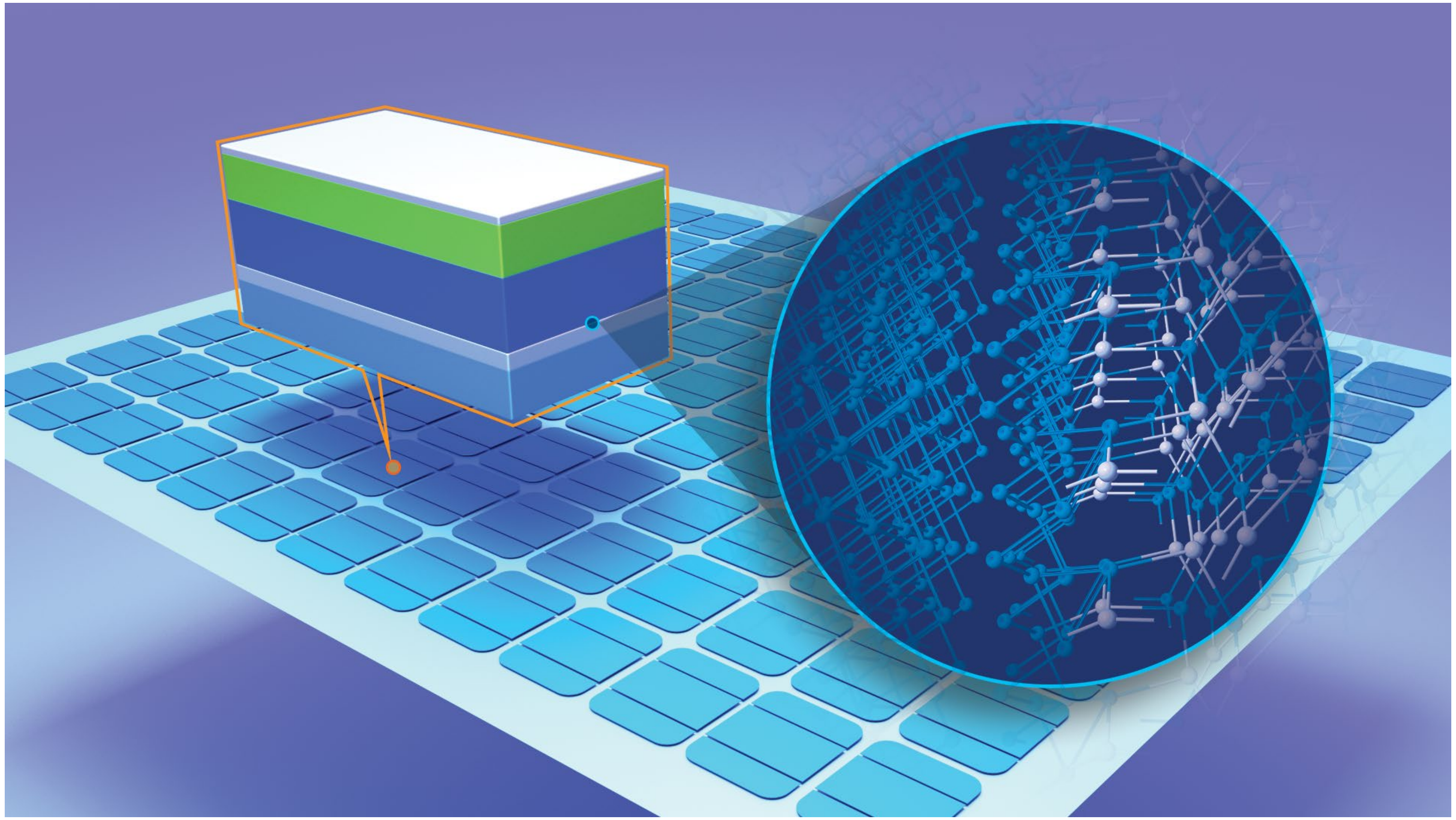
Finite-temperature photocurrent simulations using QuantumATK

Photocurrent in a silicon p-n junction – including temperature effects

Photocurrent in stacked Janus monolayers

Motivation

- Sustainable energy can be gained from solar cells.
- The efficiency of solar cell devices needs to be improved by finding materials and device concepts to achieve better control of the current generated under illumination.
- QuantumATK can be used to study new materials and devices with the aim of creating even better solar cells.



Introduction to finite-temperature photocurrent simulations using QuantumATK

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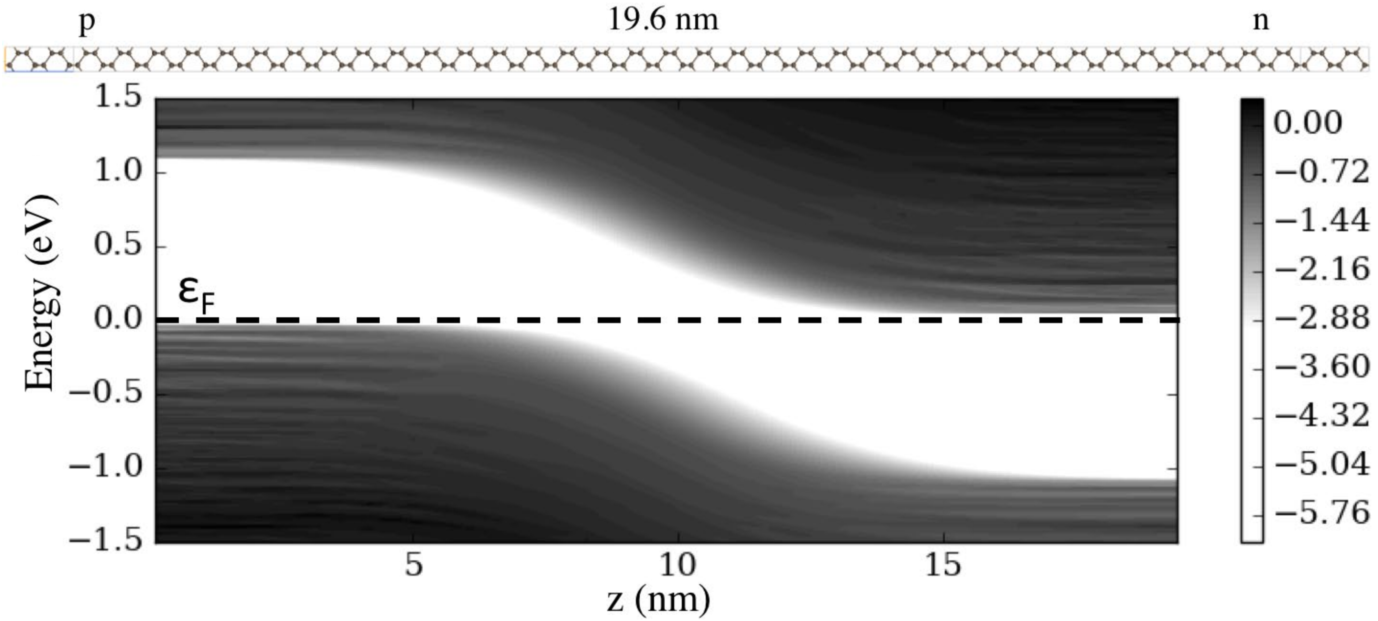
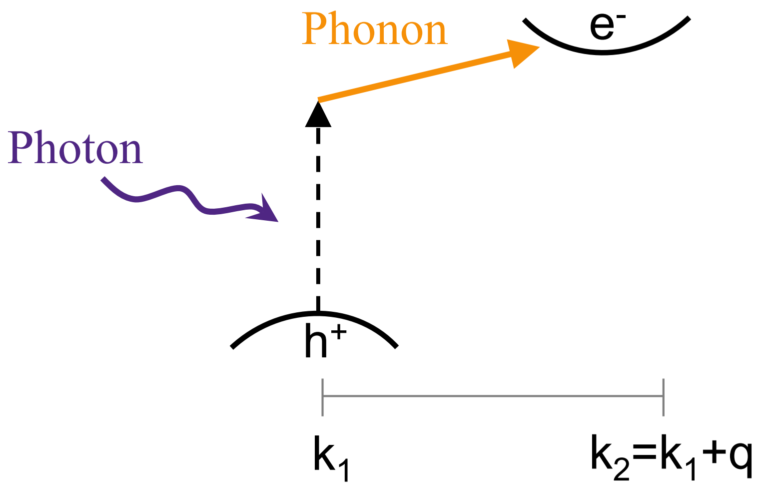
Photocurrent calculations using QuantumATK





- Photons can excite electrons from the valence band to the conduction band. Phonons are often important to include, to enable momentum transfer.
- Depending on the method, including phonons can be computationally quite demanding.

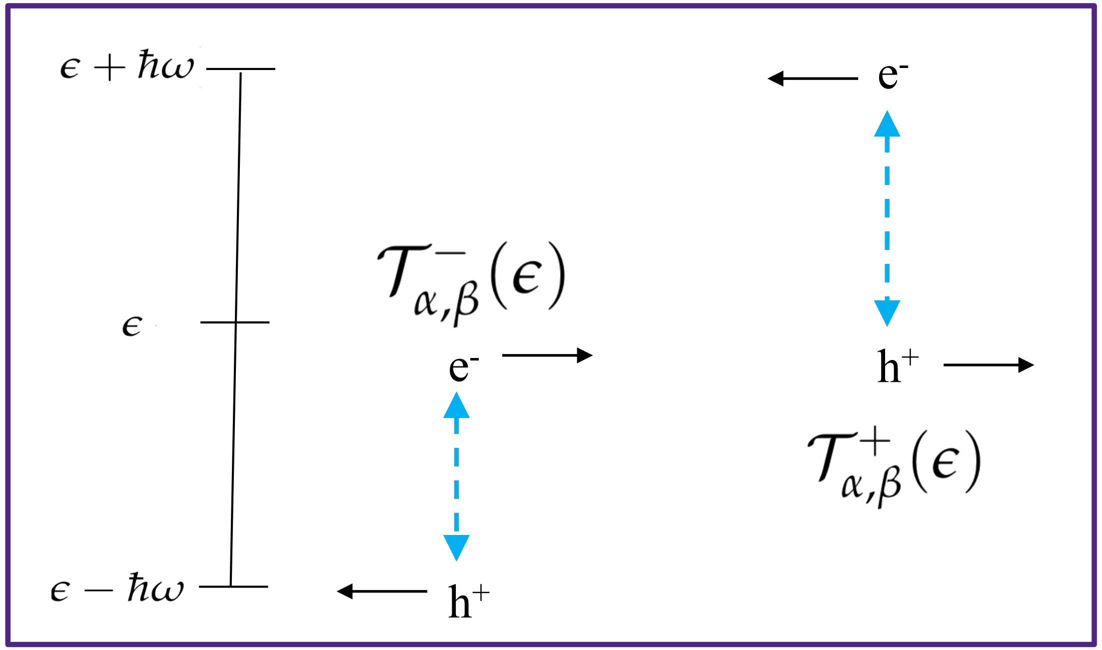
Theory

Relative permeability and permittivity

$$M_{i,j} = \frac{e}{m_0}\left(\frac{\hbar\sqrt{\tilde{\mu}_r\tilde{\varepsilon}_r}}{2N\omega\tilde{\varepsilon}c}F\right)^{\frac{1}{2}} \mathbf{e}\cdot\mathbf{p}_{ij}$$

Flux

Polarization



$$I_{\omega,\alpha} = \frac{G_0}{e}\int_{-\infty}^{\infty} d\epsilon\, [\mathcal{T}^{-}_{\alpha,\beta}(\epsilon) - \mathcal{T}^{+}_{\alpha,\beta}(\epsilon)],$$

Fermi's golden rule!

Photon energy

$$\mathcal{T}^{-}_{\alpha,\beta}(\epsilon) = N[1 - f_\alpha(\epsilon)]f_\beta(\epsilon - \hbar\omega)\mathrm{Tr}\{\mathbf{M}^{\dagger}\tilde{\mathbf{A}}_\alpha(\epsilon)\mathbf{M}\mathbf{A}_\beta(\epsilon - \hbar\omega)\}$$

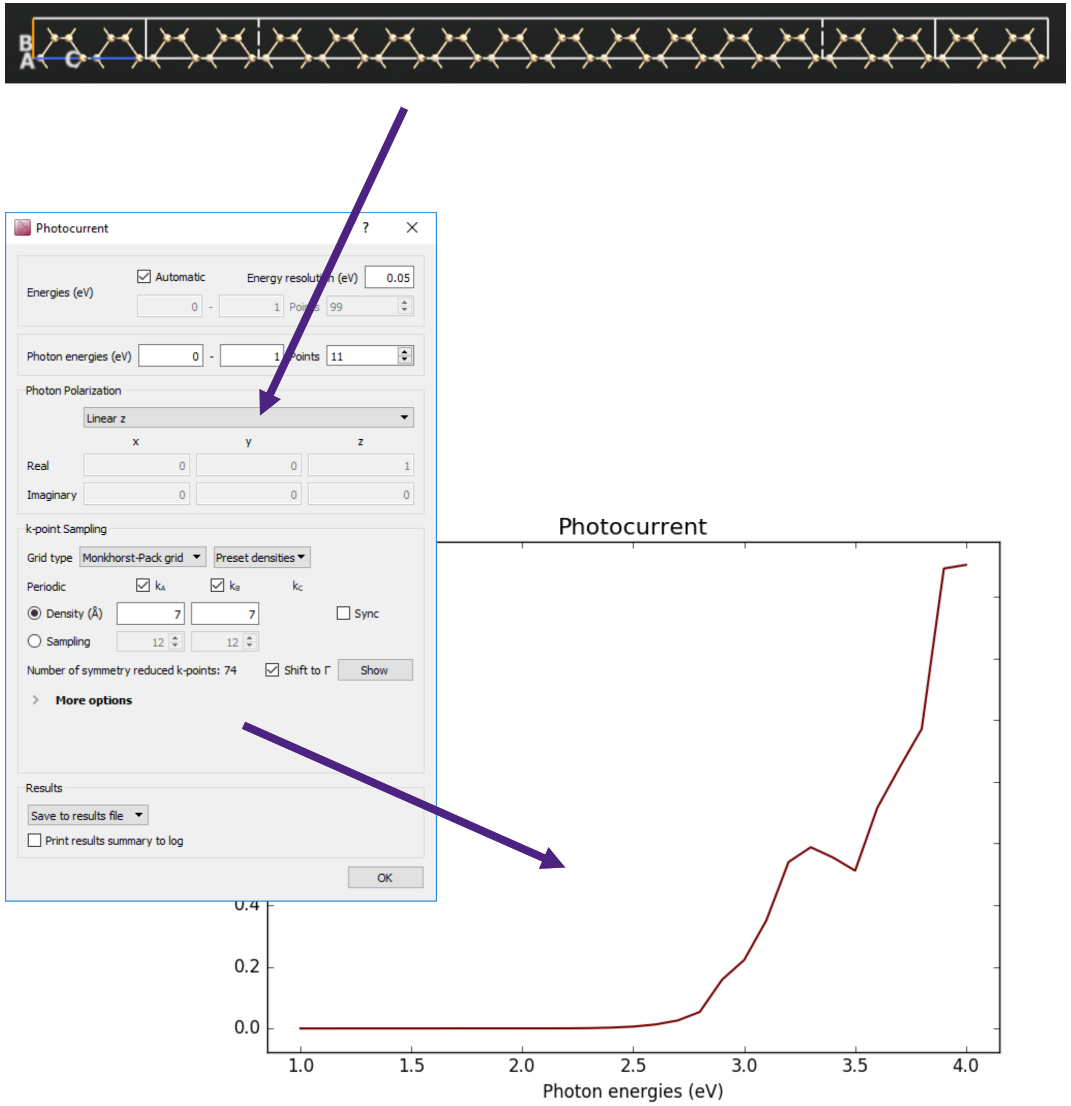
$$\mathcal{T}^{+}_{\alpha,\beta}(\epsilon) = Nf_\alpha(\epsilon)[1 - f_\beta(\epsilon + \hbar\omega)]\mathrm{Tr}\{\mathbf{M}\tilde{\mathbf{A}}_\alpha(\epsilon)\mathbf{M}^{\dagger}\mathbf{A}_\beta(\epsilon + \hbar\omega)\}$$

Energy

DOS

Photocurrent in QuantumATK

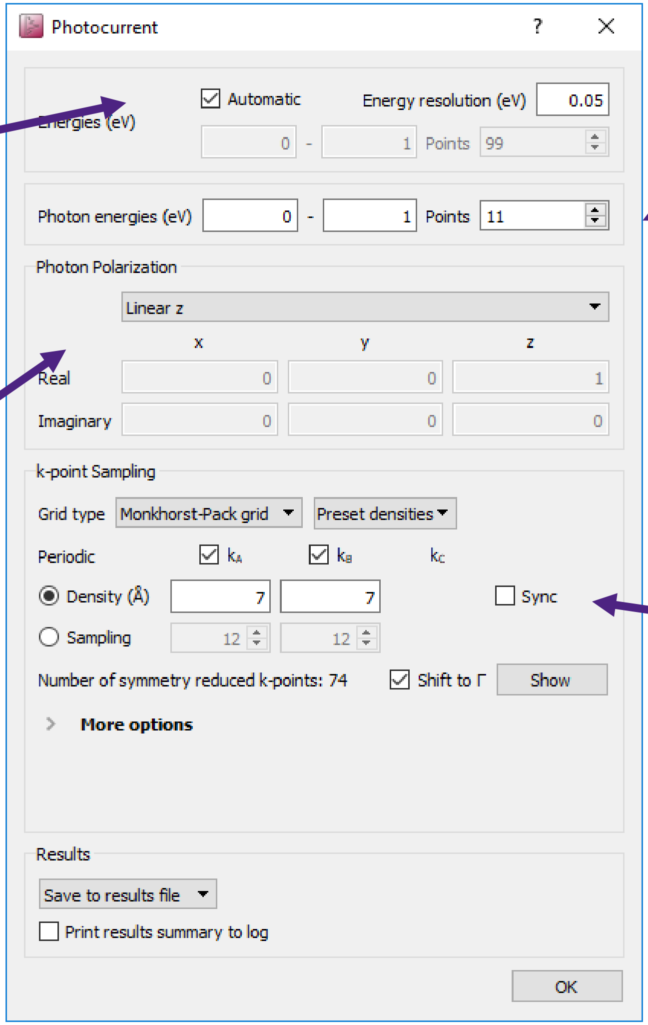
- The Photocurrent Analysis object calculates the spectral photocurrent under illumination for any device structure and combination of materials, using atomic-scale methods.
- Allows you to study the effect of:
  - Photon flux
  - Relative permeability
  - Relative permittivity
  - Photon polarization and energy



The photocurrent analysis object

Energy range taken into account for transitions. Minimum should be below the lowest electrode Fermi level and the maximum should be above the photon energy maximum.

Polarization of the photons.

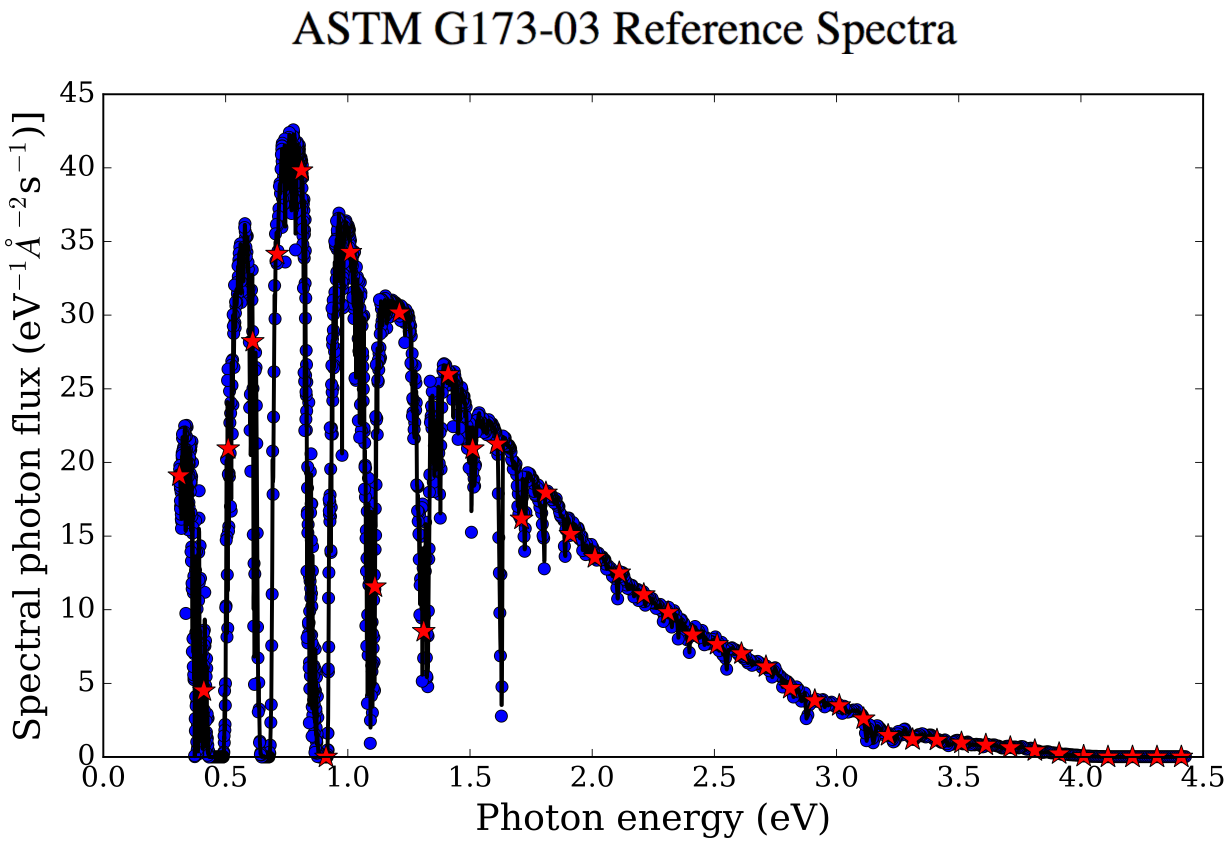


Sampling of photon energies. Governs the resolution when calculating a photocurrent spectrum.

K-point sampling used when calculating the possible transitions.

How to set up the calculation

Photocurrent calculations in devices using QuantumATK



- Spectral photon flux of sunlight can be used in calculation of a total photocurrent.
- The flux from the spectrum is used to calculate a photocurrent spectrum, which is then integrated over photon energies.

$$I_{\text{sun}}(V,T) = \sum_{\omega} I_{\omega}(F(\omega),V,T).$$

Analyzing the Photocurrent

Calculating the total photocurrent

Photocurrent in a silicon p-n junction

- Including temperature effects

Including thermal effects in QuantumATK using the Special Thermal Displacement

- The Special Thermal Displacement method allows inclusion of thermal effects using a single special configuration where the atoms are displaced according to:

$$u(T) = \sum_{\lambda} s_{\lambda}(-1)^{\lambda-1}\sigma_{\lambda}(T)$$

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First-principles electron transport with phonon coupling: Large scale at low cost

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- The special thermal displacement has been generalized to device configurations.
- Uses a single special displacement to account for the effect of temperature on the electronic structure.
- Works in the adiabatic limit (electrons decoupled from phonons).
- It can be applied to large systems where subsequent modes are approximately degenerate.

Check our webinar at https://docs.quantumwise.com/webinars/webinars.html:
"How to include electron-phonon scattering effects in large scale atomistic device simulations"

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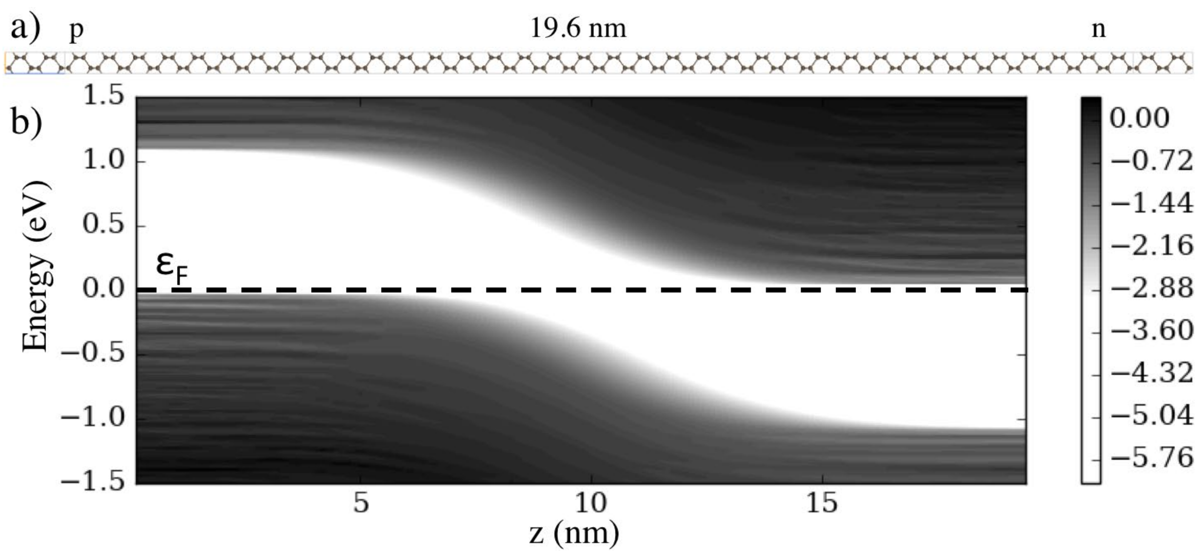
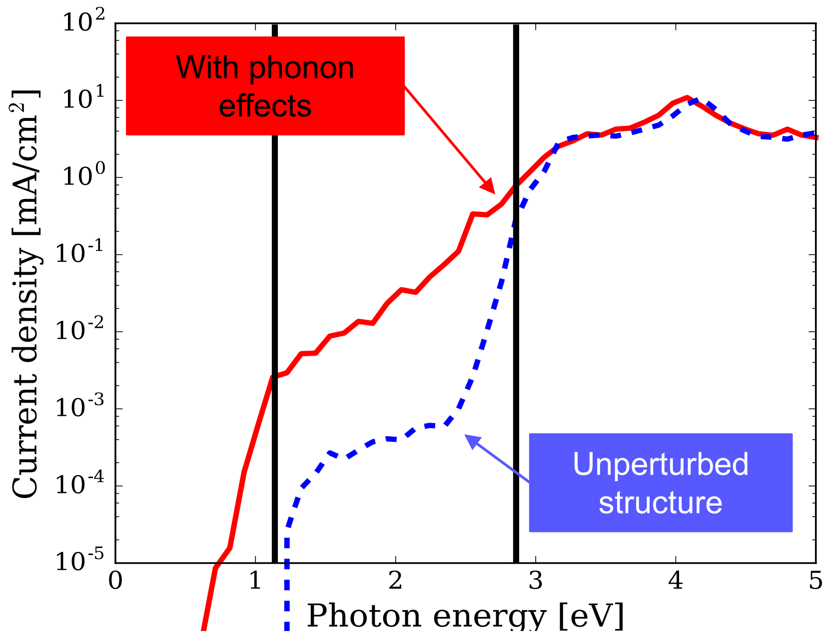
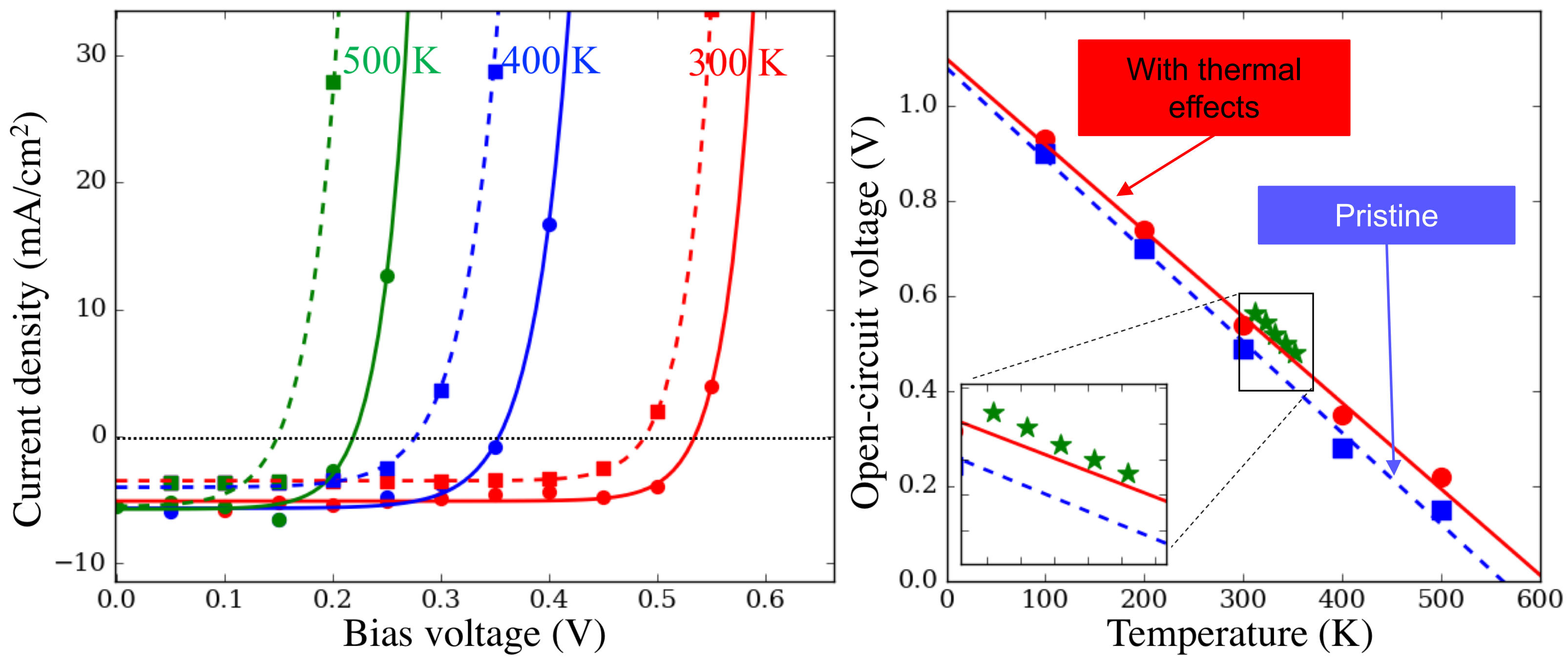
Combining Special Thermal Displacement and Photocurrent capabilities in QuantumATK





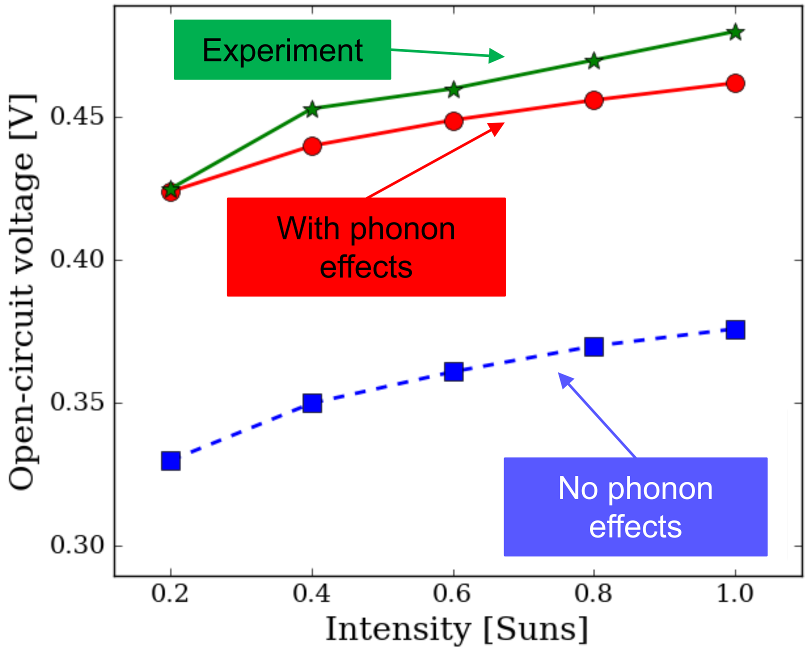
- The Special Thermal Displacement method is applied to a device configuration to calculate the photocurrent density upon illumination, including the effect of phonons.
- The calculated photocurrent shows clear onsets of photocurrent at the bandgaps, as expected.
- The direct transition is almost unaffected when accounting for the effect of electron-phonon coupling.
- There is a finite current from indirect transition even without accounting for electron-phonon coupling, unlike bulk case.

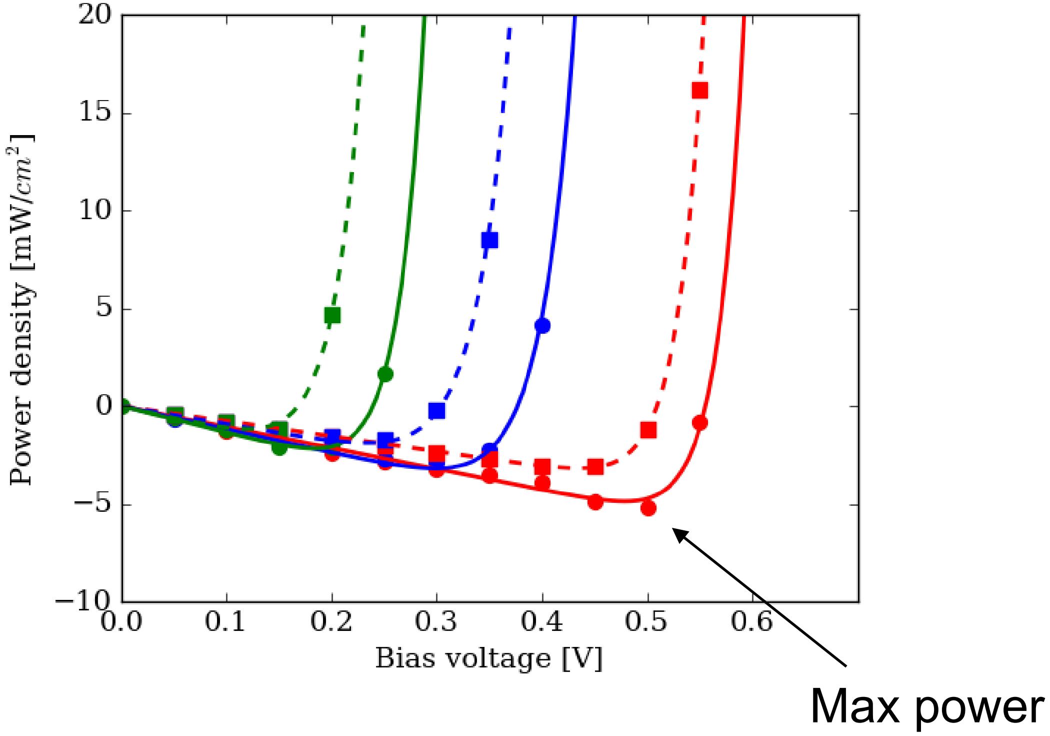
Solar cell device



- IV-curves of the illuminated device as a function of temperature - it can be seen that the electron-phonon coupling becomes more important for higher temperatures.
- From the calculations, it is possible to extract the open-circuit voltage as a function of temperature and fit it with a linear regression.
- The open-circuit voltage calculated with phonon effects results in a better agreement between the calculated results and the experimental reference.

Solar cell device

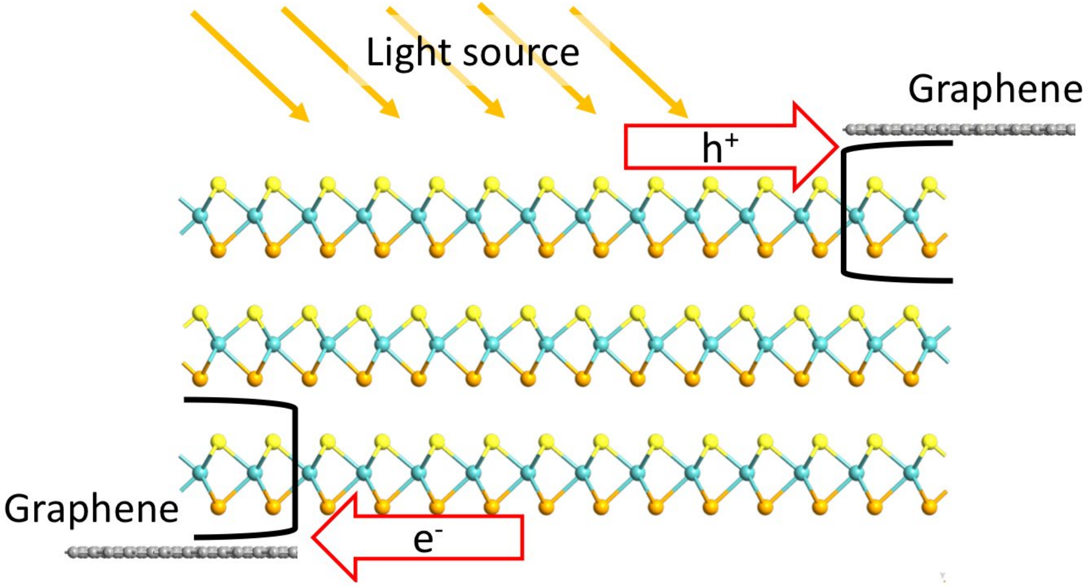


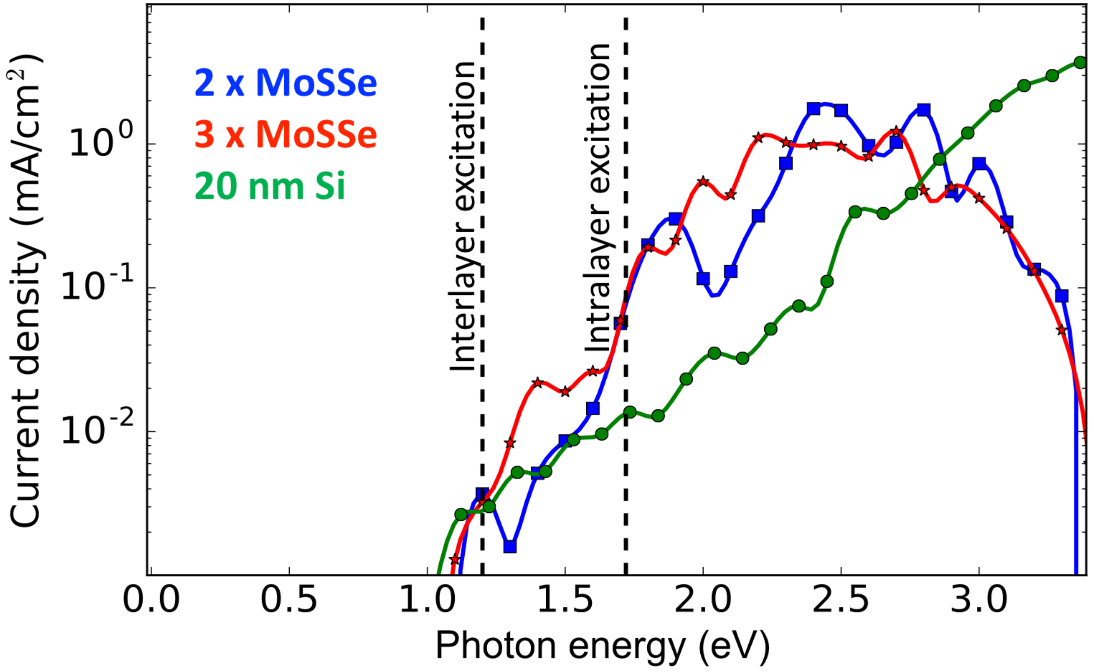


- At ideal operating voltage (0.5V) predicted maximum power: 5.14mW/cm^2.
- Max power voltage without accounting for EPC: 0.4V.
- Calculated efficiency: 2%.

Photocurrent in stacked Janus monolayers

Solar cell device





- An higher photocurrent than silicon is calculated for frequencies up 2.75 eV.
- Absorption below monolayer bandgap.
- Photocurrent changes sign at high frequencies.

Ref: M. Palsgaard, T. Gunst, T. Markussen, K. S. Thygesen, and M. Brandbyge, *"Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels"*, Nano Letters Article ASAP, DOI: 10.1021/acs.nanolett.8b03474

Further reading

- Documentation:
  - Tutorial: https://docs.quantumwise.com/tutorials/photocurrent/photocurrent.html
  - Manual: https://docs.quantumwise.com/manual/Types/Photocurrent/Photocurrent.html

- Literature:
  - M.Palsgaard, T. Markussen, T. Gunst, M. Brandbyge, and K. Stokbro, "*Efficient First-Principles Calculation of Phonon-Assisted Photocurrent in Large-Scale Solar-Cell Devices*", Phys. Rev. Appl. 10, 014026 (2018).
  - M. Palsgaard, T. Gunst, T. Markussen, K. S. Thygesen, and M. Brandbyge, *"Stacked Janus Device Concepts: Abrupt pn-Junctions and Cross-Plane Channels"*, Nano Letters Article ASAP, DOI: 10.1021/acs.nanolett.8b03474

Thank You

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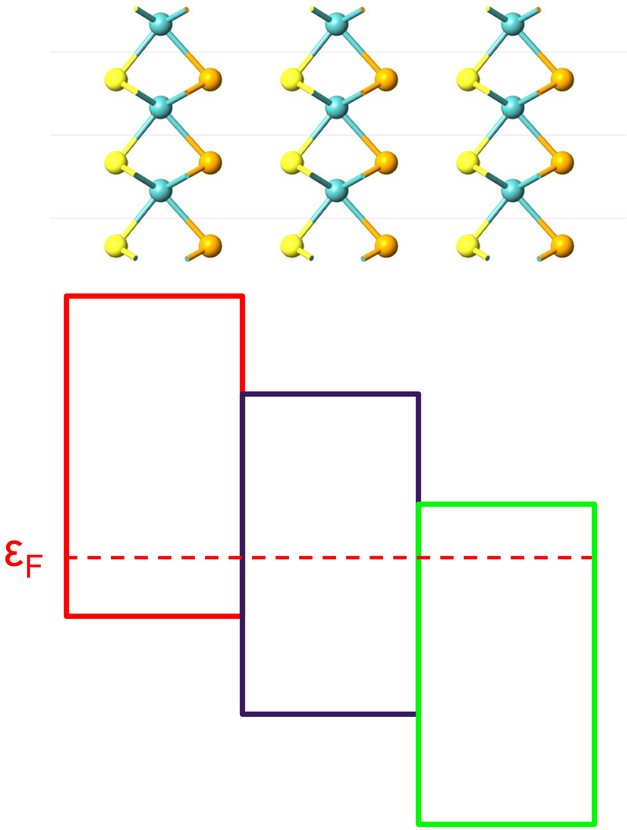
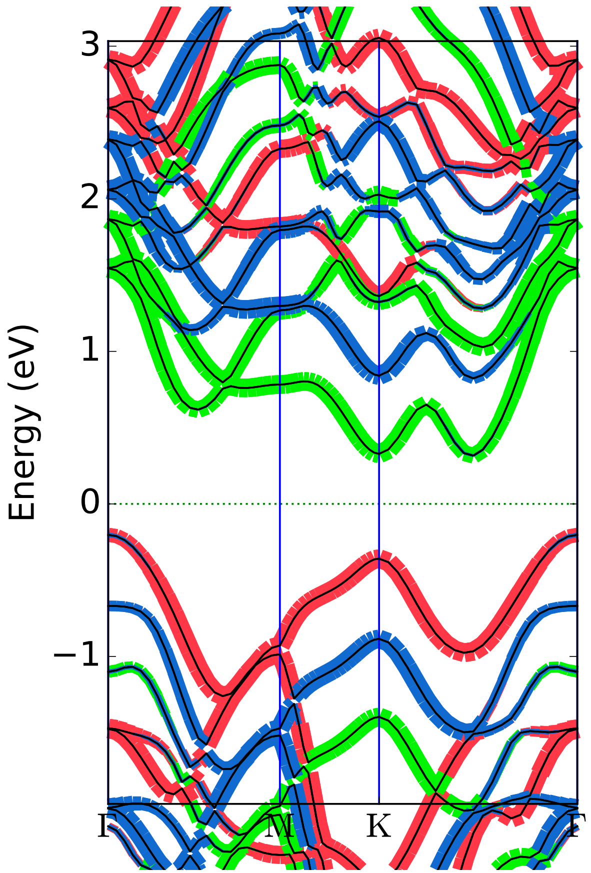
Stacking dipoles





- Stacking the individual Janus monolayers one on top of the other leads to the formation of a *p-n* junction due to the increase in the built-in electric field.

