Detailed Technical Specification

Specifications for OPV/ PEROVSKITE SOLAR CELL / OLED simulation software

Software should have the following capabilities:-

1. Software should be specifically designed for one dimensional optical and electrical modeling of semiconducting devices and particularly for designing OPV/PEROVSKITE/Organic LEDs Devices.

2. Modeling charge transport & recombination in organic semiconductors preferably with Drift Diffusion equations.

3. Must provide advanced device physics: quenching, excitons, traps, doping, AC & transient responses.

4. Must generate I-V-curves, impedance spectroscopy and transient responses (including photo-CELIV).

5. It should have State-of-the-art mobility models such as Poole Frankel, EGDM/ECDM, constant mobility.

6. Must address conductive doping, charge trapping, Injection properties of the contacts as well as exciton recombination, generation, quenching and roll-off diffusion.

7. Provision for ionic contribution & hysteresis effect to simulate perovskite solar cell & light-emitting electrochemical cells.

8. Should have capability of DC, AC & Transient Simulation with transient solver method like runge kutta, Emplicit Euler, Adaptive runge kutta, Enable transient temperature.

9. Must have built-in Impedance solver which calculates equivalent impedance & capacitance.

10. It should have easy to use Graphical User Interface with these features:-
- **a.** Intuitive access to device structure, material parameters, working files, simulation output.
- **b.** Optimization Toolbox to maximize the device efficiency.
- **c.** Sweep function to analyze influence of material parameters on the device efficiency.
- **d.** Easy access to a library of simulation examples and material property database.
- **e.** Key graphs should be automatically generate & export for large area OPV/OLED software.
- **f.** Results should be exported to a number of different file formats like excel, png, pdf, svg, txt etc.
- **g.** It should be fully compatible with Python.

11. It should be capable of simulating experiments like transient electroluminescence (TEL), dark injection transient (DIT), CELIV, exciton decay rate.

12. Reproduce, quantify and understand the influence of these different effects from the comparison between the simulated and experimental characteristics of the device.

13. Fully coupled steady-state, AC (Impedance), IMPS and transient modeling.

14. Understand device operation from electronic and ionic charge profiles.

15. Software should support UNLIMITED Semiconductor Layer.

16. It should be designed scattering layers and optimize OPV/OLED efficiency with these features.
- Simulation of scattering by structured electrodes (external scattering)
- Scattering by nanoparticles in the bulk (internal scattering) by using Mie theory.
- Import rough surface textures from profilometric data or use the synthetic rough surface
- Combine multiple scattering layers within the same device.
- Scattering Particles micro or nano particles dispersed in a host material
- Optimize concentration and refractive index of particle scattering layers.
- Simulate the effect of the particle size distribution & spherical particles of any size.
- Combine stack and incoupling, outcoupling layer design.
- Import experimental AFM & BSDF data.
- Microlenses and -textures via ray-tracing, geometric (ray) or physical (wave) optics.

17. Software must have absorption module for OPV/Perovskite Solar cell with these feature.
- It allows you to maximize light absorption in the device.
- Optimize the combination of the different layer thickness in your stack,
- Adjust and match the short-circuit currents, Open circuit voltage, Fill factor of solar cells.
- Compute absorbance of each specific layer & total device in the solar cell.
- Reflectance, transmittance, absorbance spectra, polarization, Quantum Efficiency.
- Spectral penetration of external illumination light.
- Calculation of the maximum power point with a coupled optical and electrical (drift-diffusion) simulation.

18. Multithreading ensuring high speed computation & Fitting with optimization algorithms should be included.

19. The software package should be able to be installed in both Windows & Linux Operating System.

Requirement for OPV/PEROVSKITE/OLED simulation:

1. It should simulate OLEDs from charge injection to light extraction, Absorption for OPV devices.

2. Analyze optical emission spectra and wave-guided mode contributions with the suitable module.

3. Design isotropic, transparent, incoupling & out-coupling layers for efficiency and color stability.

4. Predict the light emission characteristics of an OLED by using dipole emission model. Several device properties should be modeled such as:
   a. Electroluminescence emission pattern.
   b. Micro-cavity effects by thin film optics.
   c. Photophysical properties such as efficiency, angular color, and brightness changes.
   d. Excitonic processes in OLEDs, by combining optical and electrical simulation.
   e. Waveguided and plasmonic modes, quenching, distribution, and orientation of the emitters.

5. Must calculate the current-voltage (IV) characteristics, charge concentration, electric field and recombination zone of OLEDs devices/OPV/Perovskite Solar cells.

6. Should be able to calculates IV curve of OLEDs/ OPV/Perovskite Solar cells using suitable physical models and considering mobility, charge traps, doping, recombination & illumination.

7. Model different excitonic processes such as recombination & dissociation of electron-hole pairs, exciton diffusion, radiative & non-radiative decay, triplet-triplet interaction in OLEDs.

8. Model energy transfer between different exciton states, as in Thermally Activated Delayed Fluorescence(TADF) emitters, Exponential DOS, Gaussian DOS & Single Energy level.

9. Should simulate radiative decay and light emission including Purcell quenching effects, Doping & Trapping effect.

10. Should be able to calculate the optimal thickness of absorbing layer for OPV/Perovskite solar cell.

11. Simulate effect of mobile anions and cations on OLED/OPV/Perovskite device characteristics.

12. Generate charge, recombine Hopping between different states at interface for operation of OLEDs/ OPV/Perovskite Solar cell.

13. Software should have emission module for mode analysis for OLED application.

14. Scattering by particles, Gaussian, mono dispersion mode, poly dispersion mode, Radius, refractive index.

15. Scattering by different type model like Lambertian, phong, Gaussian, Fourier, 3D Ray tracing.

16. RMS Setting: Defines the roughness of the interface to calculate the Haze. Define diffusion length top & bottom for interface.

17. Software should have provision to enable electrical circuit series resistance, parallel resistance, parallel capacitance, lateral resistance, device voltage residuum etc.

18. Should be able to display transmission or reflection of incident light for coupled absorption-emission simulations

19. Software should be dongle based license.

IMPORTANT: Unlimited updation of patches and bug fixes must be offered within maintenance & support period.