The influence of injection barriers on performance of organic solar cells studied by drift-diffusion model with transport layers

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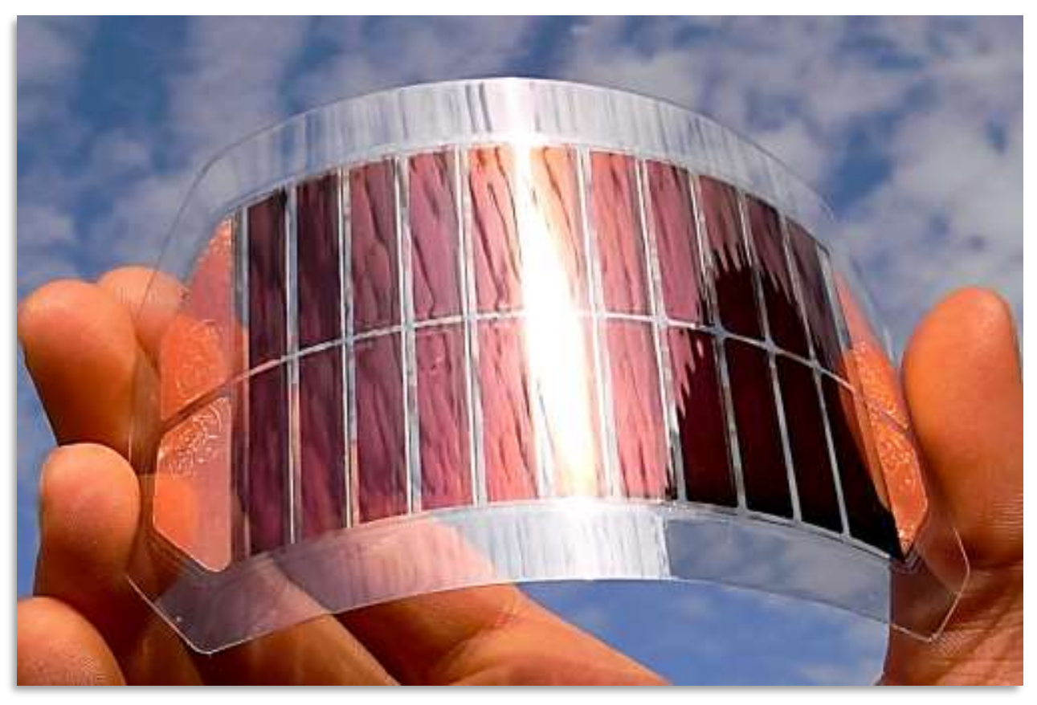
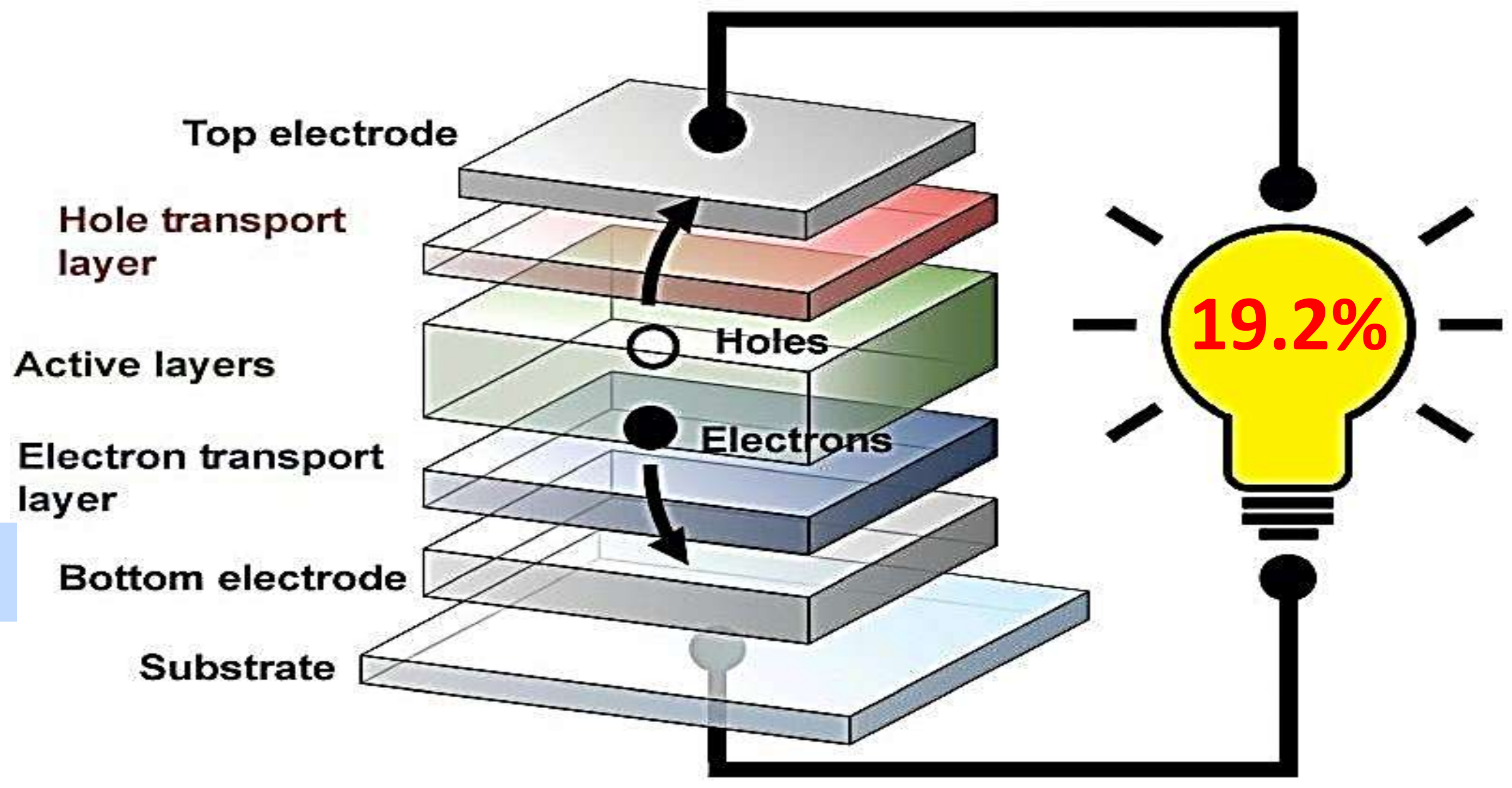
Motivation



Theoretical explanations needed!

Comprehensive **drift-diffusion model (DDM)** should be developed

- low-cost,
- lightweight,
- flexible,
- ideal for roll-to-roll large-scale processing...



Transport layers are not included in current DDMs

Drift-diffusion model

- ϕ - electrostatic potential
- q - elementary charge,
- n and p - electrons and holes densities
- D_n and D_p - electron and hole diffusion coefficients
- G is generation term described by Beer-Lambert law

Continuity equations:

$$-n(x)\cdot\mu_n\cdot\frac{\partial^2\varphi(x)}{\partial x^2}-\mu_n\cdot\frac{\partial\varphi(x)}{\partial x}\cdot\frac{\partial n(x)}{\partial x}+D_n\cdot\frac{\partial^2 n(x)}{\partial x^2}=R-G$$
$$-p(x)\cdot\mu_p\cdot\frac{\partial^2\varphi(x)}{\partial x^2}-\mu_p\cdot\frac{\partial\varphi(x)}{\partial x}\cdot\frac{\partial p(x)}{\partial x}-D_p\cdot\frac{\partial^2 p(x)}{\partial x^2}=G-R$$

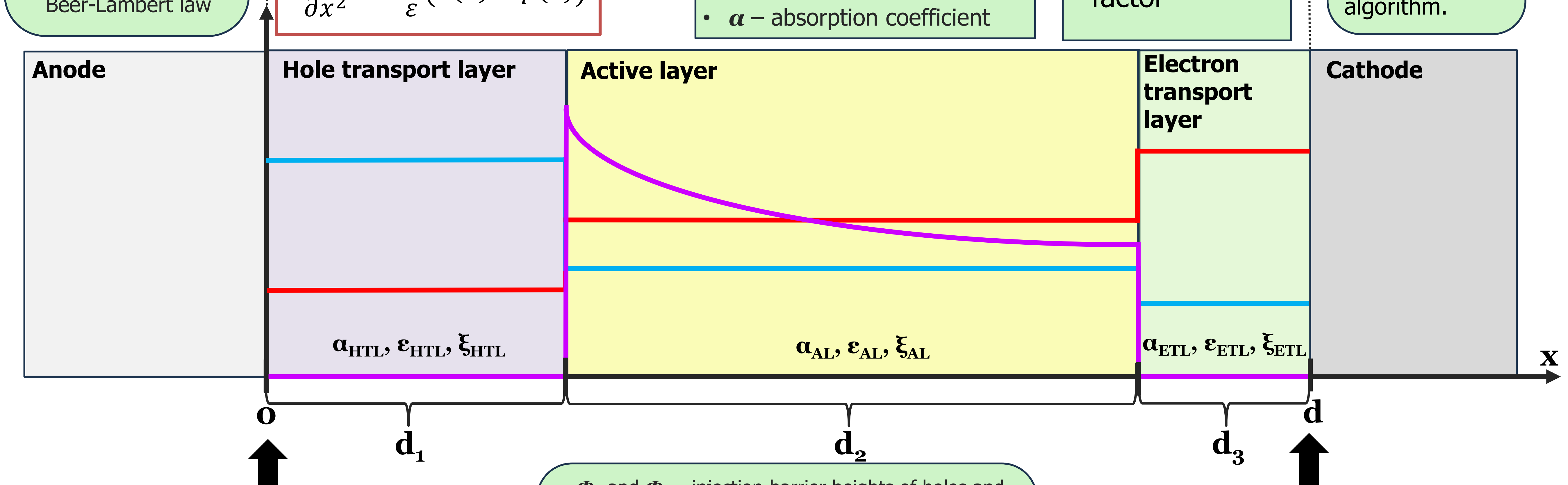
Poisson's equation:

$$\frac{\partial^2\varphi(x)}{\partial x^2}=\frac{q}{\varepsilon}(n(x)-p(x))$$

- ε – permittivity
- μ_n and μ_p - electron and hole mobilities
- α – absorption coefficient

- $R=\xi\frac{q}{\varepsilon}\frac{\mu_n+\mu_p}{2}$ - reduced Langevin recombination rate
- ξ – reduction factor

The system of equations was solved with use of the finite difference discretization improved by Scharfetter and Gummel approach and the Newton algorithm.



Boundary condition:

$$\varphi(x=0)=0$$
$$n(x=0)=n_{th}^{a}=N_C\exp[-(E_g-\Phi_p)/k_B T]$$
$$p(x=0)=p_{th}^{a}=N_V\exp[-\Phi_p/k_B T]$$

- Φ_n and Φ_p – injection barrier heights of holes and electrons respectively
- n_{th}^a and n_{th}^c - thermionic charge carrier densities of electrons at anode and cathode respectively
- p_{th}^a and p_{th}^c - thermionic charge carrier densities of holes at anode and cathode respectively
- N_c and N_v – effective density of states
- E_g – energy gap

Boundary condition:

$$\varphi(x=d)=V+V_{bi}$$
$$n(x=d)=n_{th}^{c}=N_C\exp[-\Phi_n/k_B T]$$
$$p(x=d)=p_{th}^{c}=N_V\exp[-(E_g-\Phi_n)/k_B T]$$

Conclusions

- A simple way of including transport layers in the DDM is presented – each layer (HTL, AL and ETL) is described with its electrical and optical parameters. Hole and electron injection barriers are considered.
- **Model validation 1.** J-V curve simulations show expected trends with changing hole/electron injection barriers.
- **Model validation 2.** Simulated J-V curves of ITO/P3HT:PCBM/Al device (structure without transport layers) reproduce the experiment well when realistic values of hole/electron injection barriers are applied in the DDM.
- **Model validation 3.** Simulated J-V curves of ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al (sturcture with transport layers) show excellent agreement with experiment when zero hole/electron injection barriers are used in the DDM – this confirmes electrodes Fermi level pinning.

Acknowledgments: This work was funded by the Serbian Ministry of Science, Technological Development and Innovations and James W. Adams endowed professorship that is made available through the State of Louisiana Board of Regents Support Funds.

Results

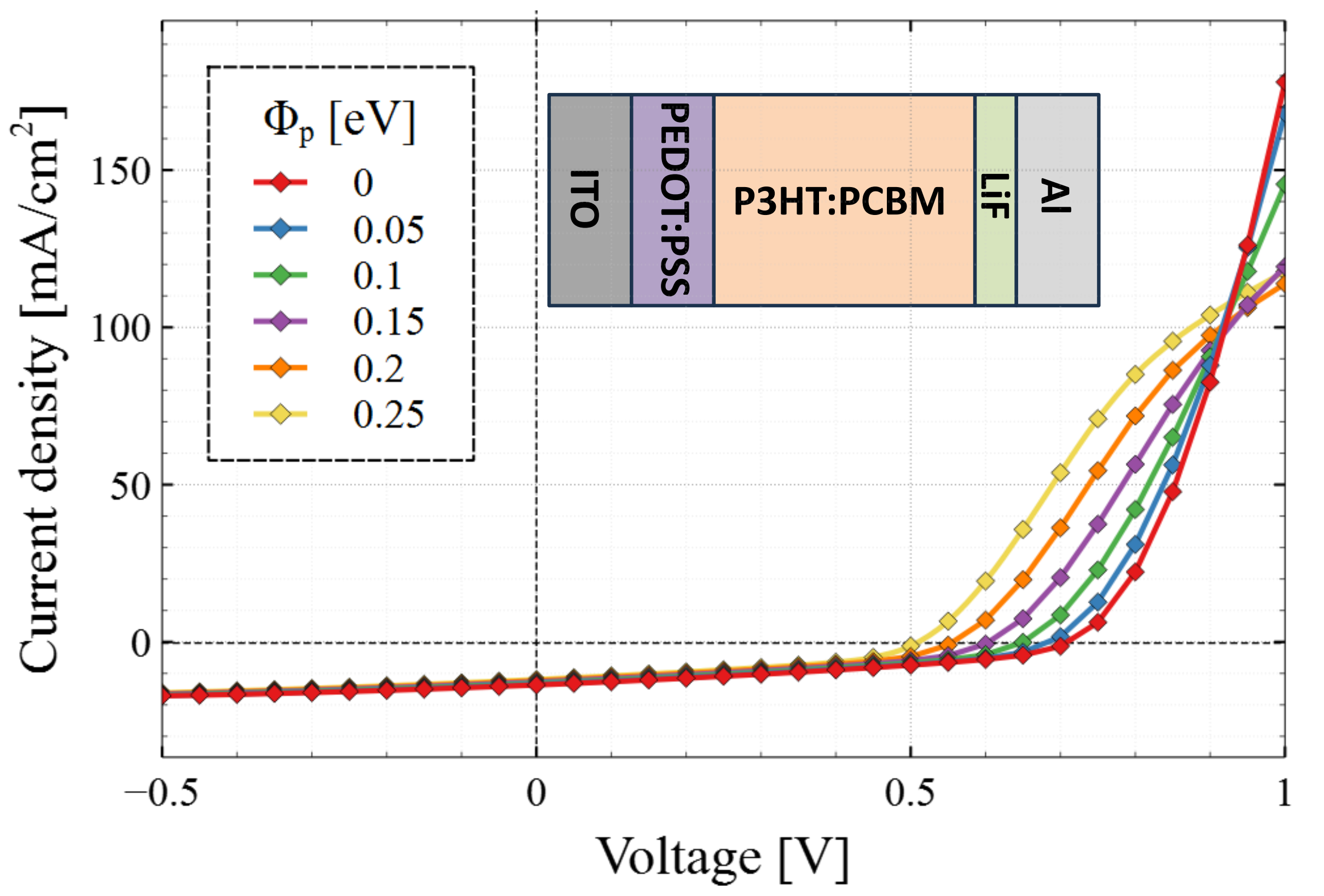


Fig. 1. J-V curves simulated for different hole injection barriers using DDM with included transport layers.

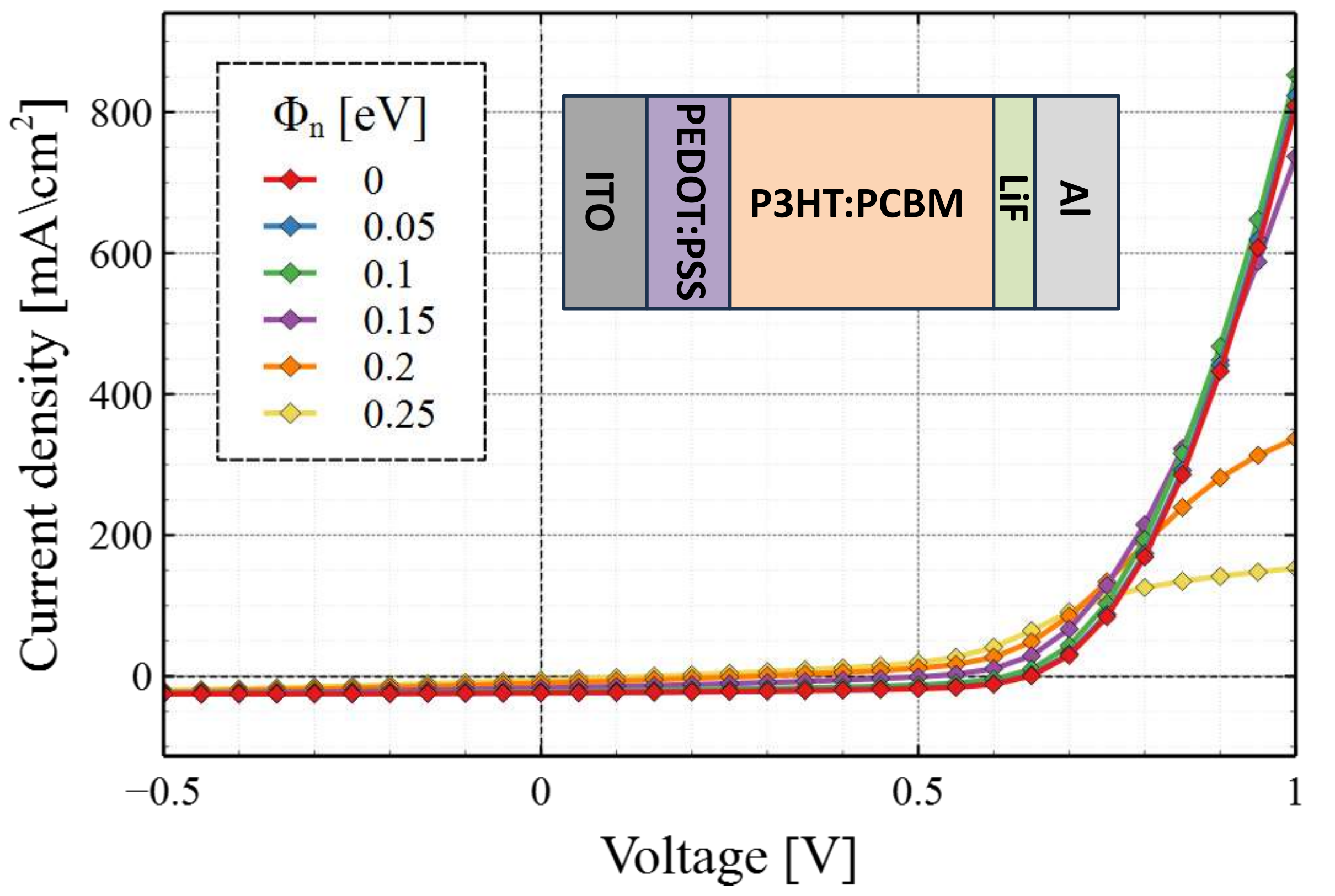


Fig. 2. J-V curves simulated for different electron injection barriers using DDM with included transport layers.

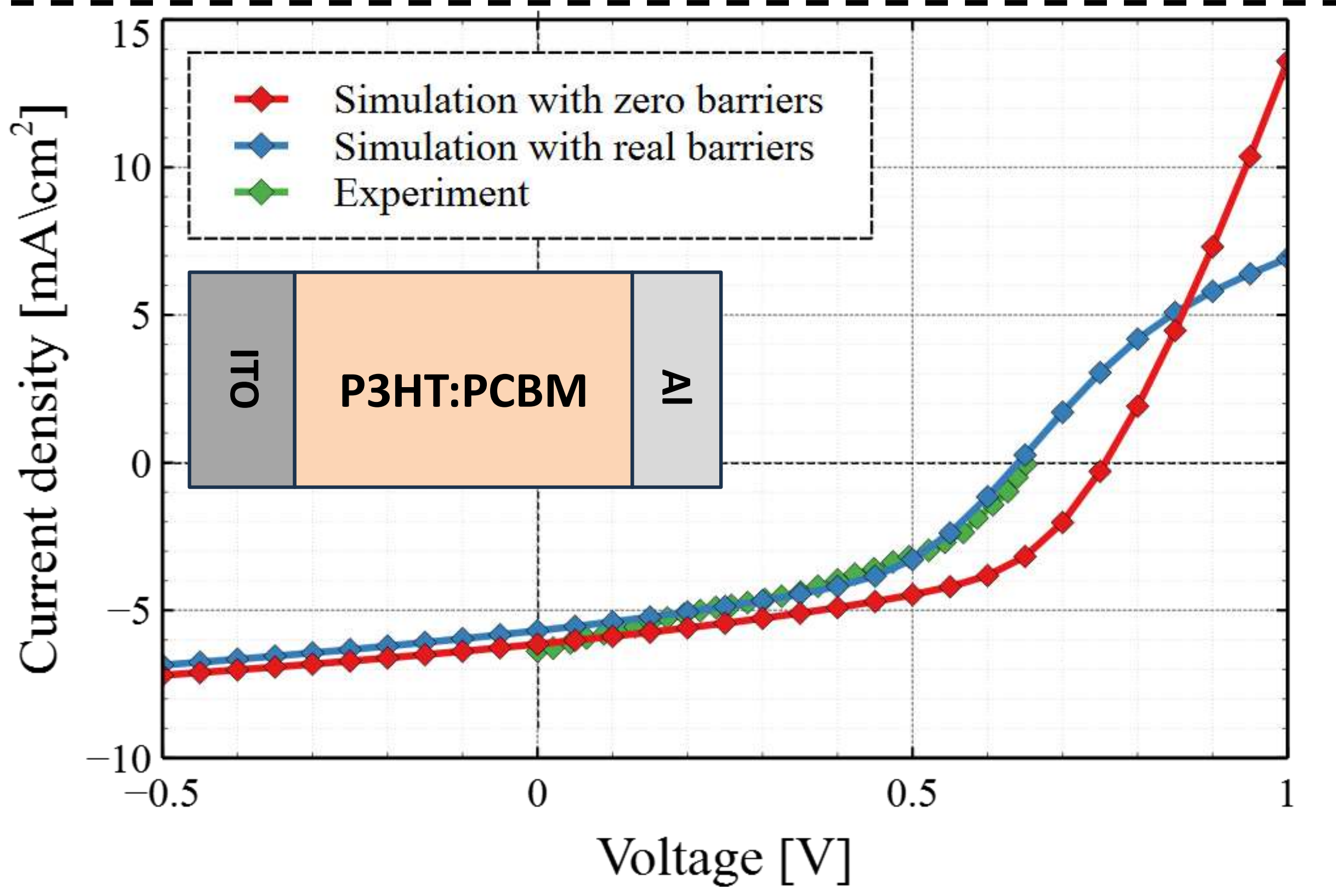


Fig. 3. Simulated J-V curves for the structure without transport layers using zero and realistic injection barrier values in the DDM compared to the measured J-V curve.

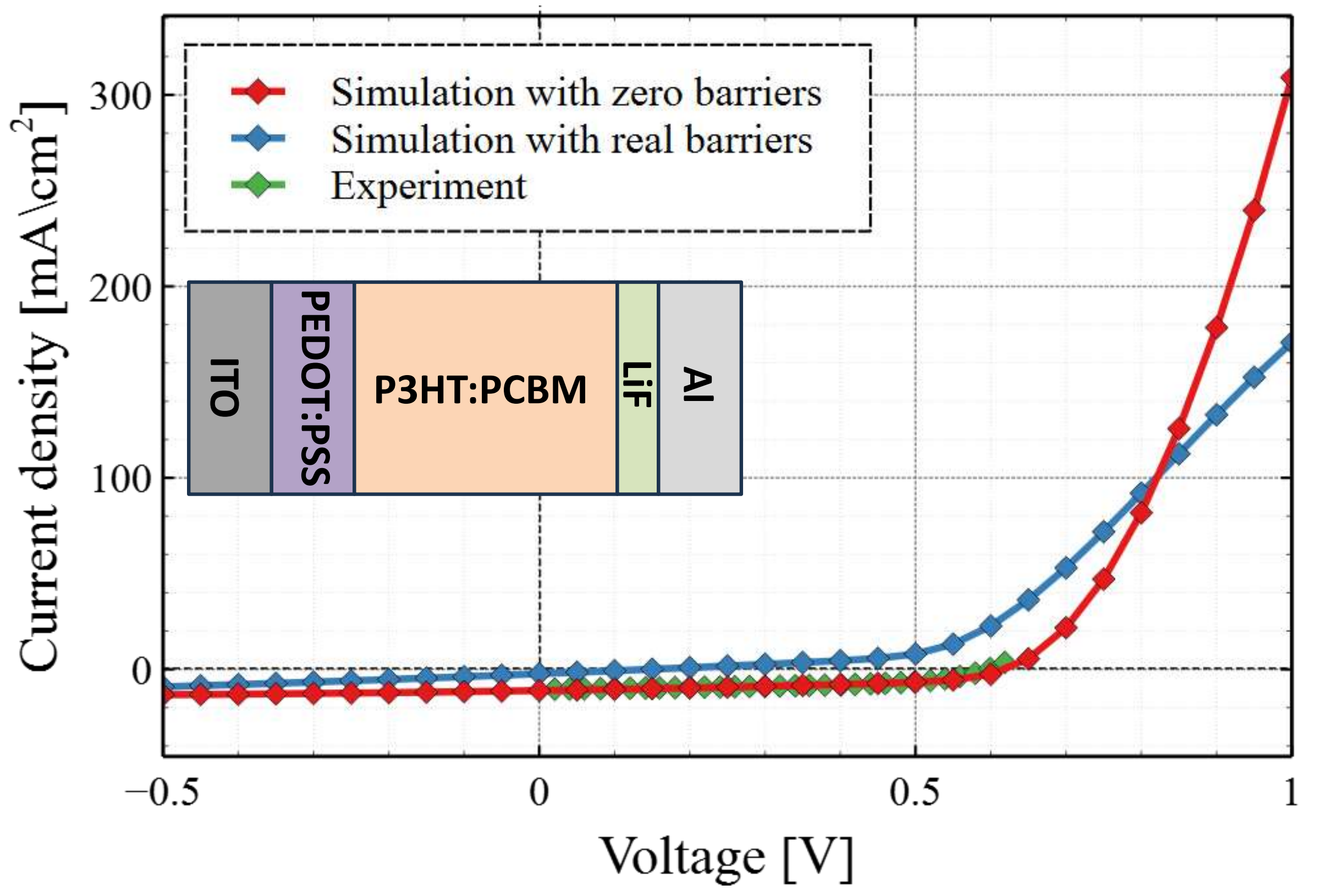


Fig. 4. Simulated J-V curves for the structure with transport layers using zero and realistic injection barrier values in the DDM compared to the measured J-V curve.