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Enhancing organic solar cell efficiency through metalloporphyrin encapsulation

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Introduction

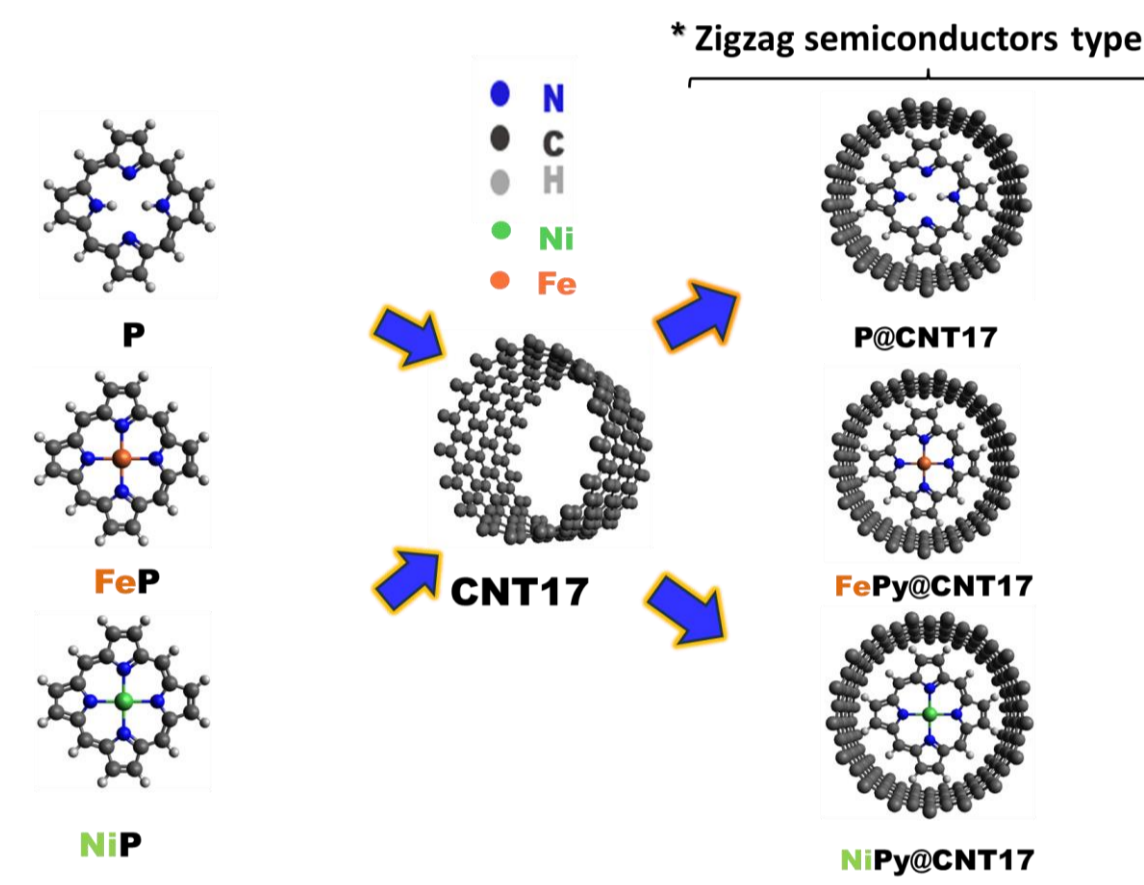
- Solar cells have evolved through three key generations. **First-generation** silicon photovoltaic (PV) cells^{1,2}, with efficiencies up to 25%, are the most widely used but are expensive. **Second-generation** thin-film PV cells offer lower costs and flexibility, though their efficiency remains limited.
- Third-generation** organic solar cells (OSCs) are attractive due to their low production costs and flexibility. However, their performance is constrained by poor absorption in the solar spectrum, limited optoelectronic tunability, low charge mobility, and thermal instability^{3,4}.

How can we overcome this issue



Methods

- First-principles density functional theory (DFT) calculations were performed using the Vienna Ab initio Simulation Package (VASP).
- Generalized Gradient Approximation (GGA) and HSE06 functionals were applied to investigate the systems..
- This system was studied across different configurations, with the frontal plane of the molecules aligned vertically in relation to the nanotube's axis.

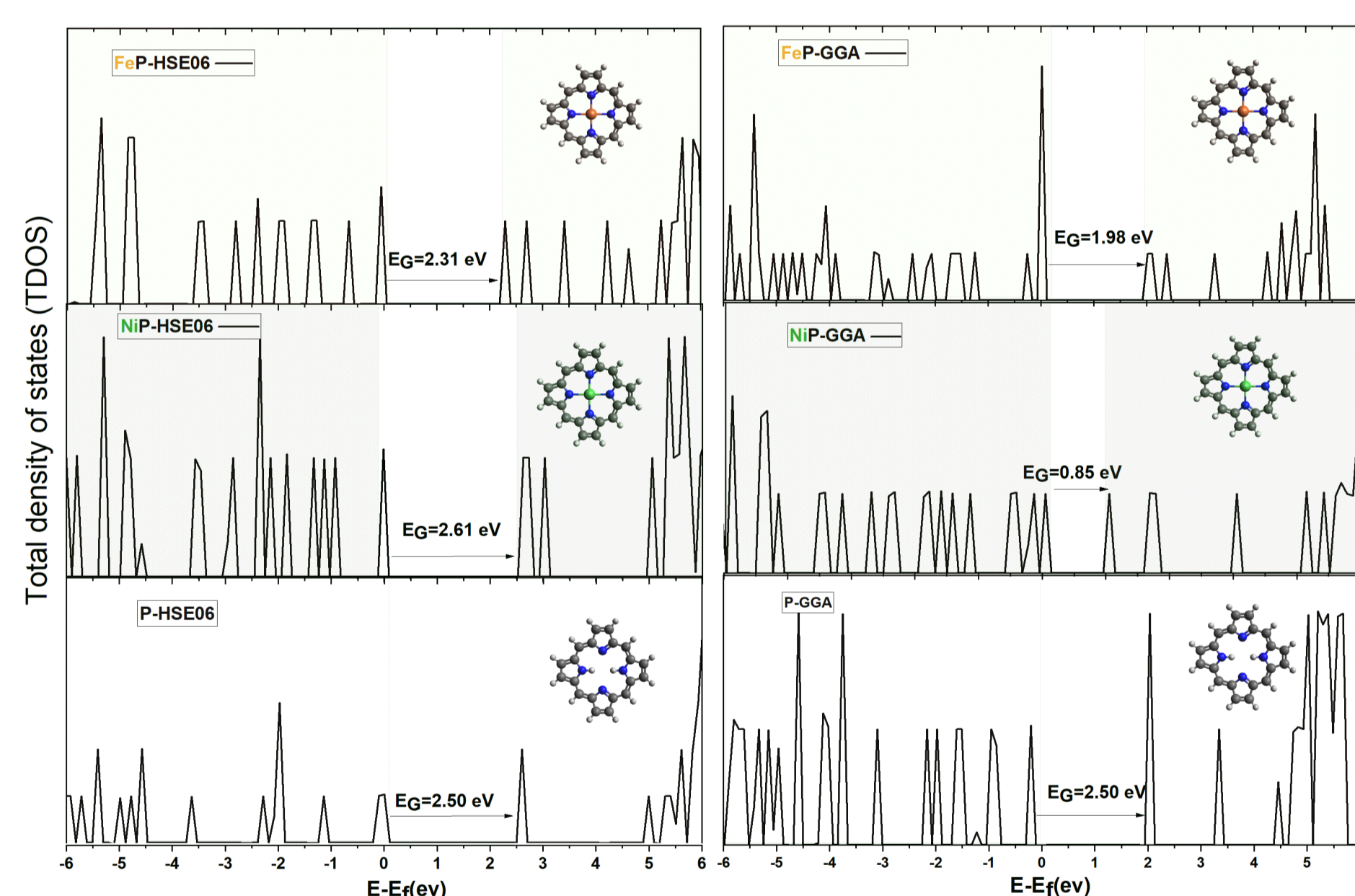


Results

Computational physical properties of metalloporphyrin molecule/ P; NiP; FeP.

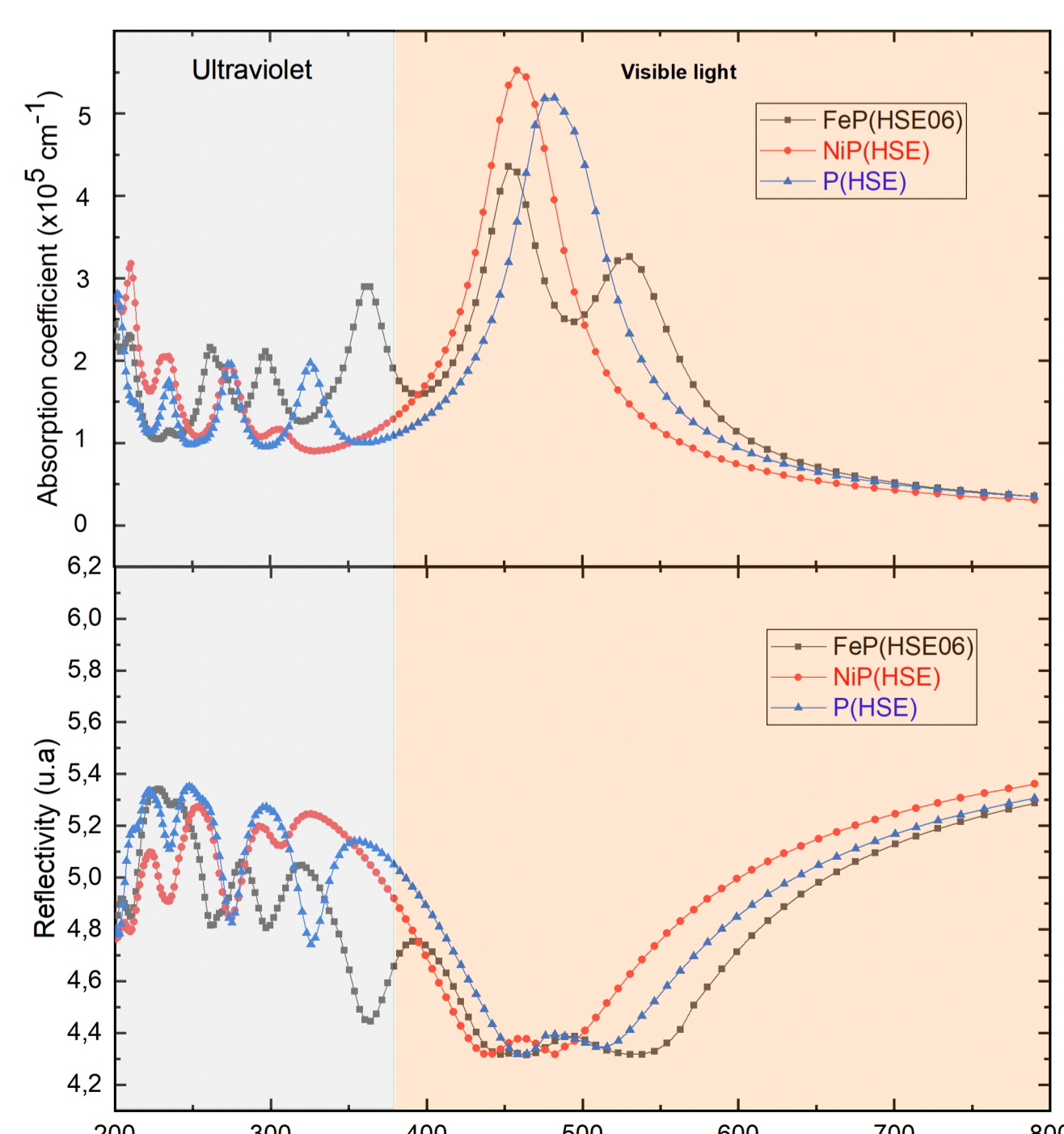
Electronic properties

- Reduction of the bandgap after incorporating metal atoms in the center of the porphyrin molecule.



Optical properties

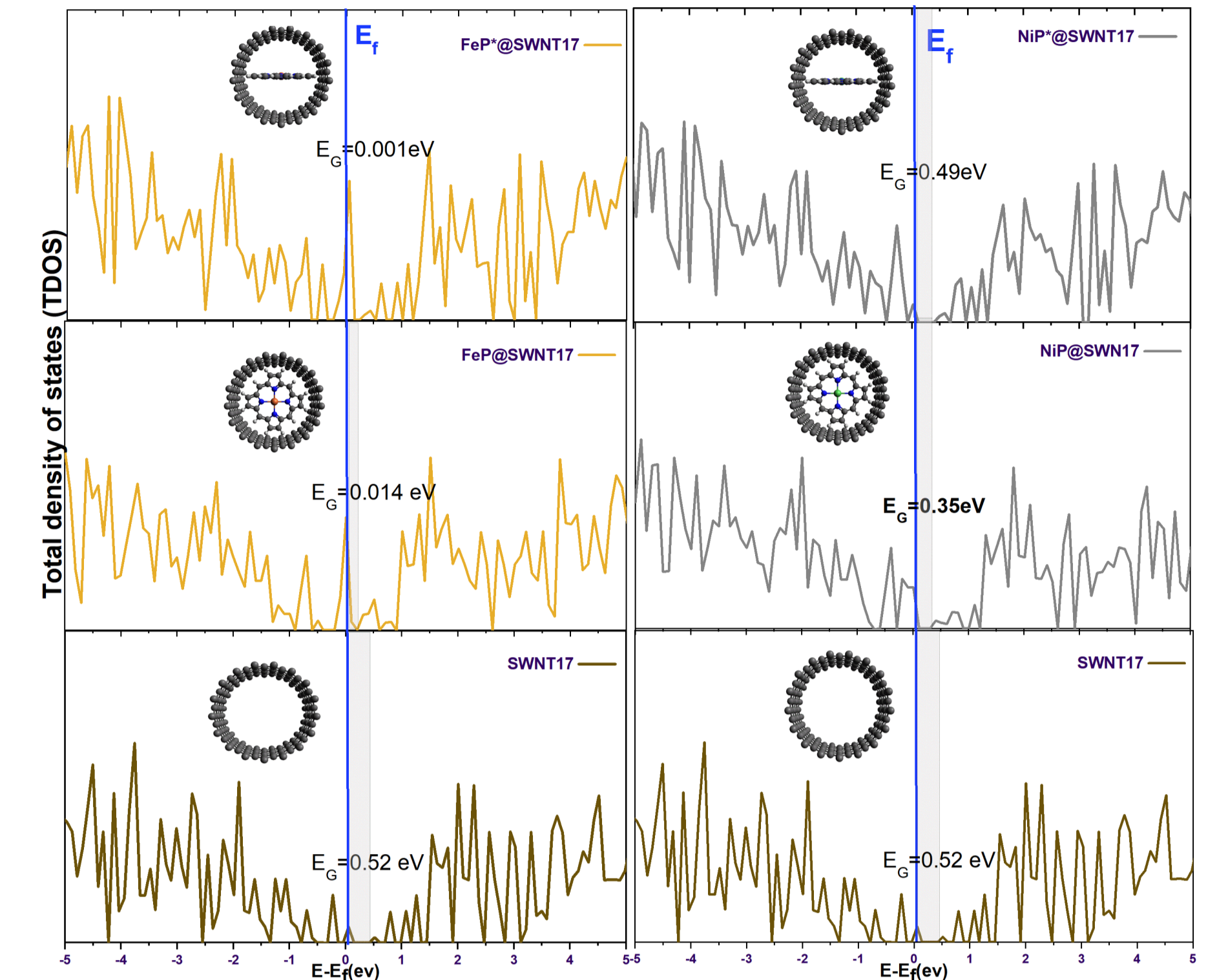
- Metalloporphyrin molecules show weak absorption in the ultraviolet (UV) region.
- Strong absorption is observed in the visible light region for Metalloporphyrin molecules.
- the UV reflectance of metalloporphyrin curves is significantly higher than that of visible-light.



Computational physical properties of encapsulated metalloporphyrin molecule within carbone nanotube/ P@SWNT17; NiP@SWNT17; FeP@SWNT17.

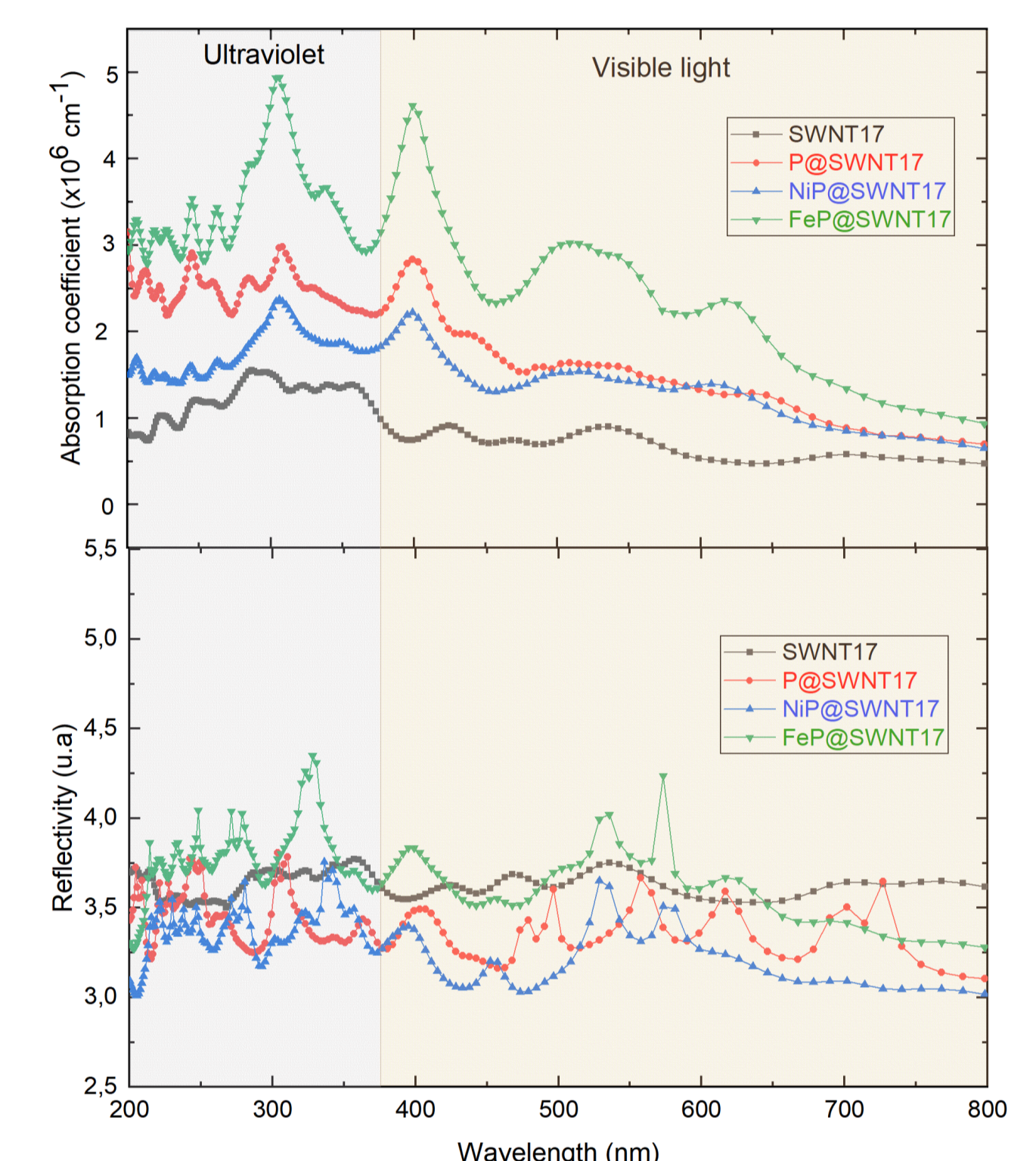
Electronic properties

- Bandgap reduction occurs after encapsulating the molecule inside the carbon nanotube.
- Indicates charge transfer from FeP or NiP to SWNT17



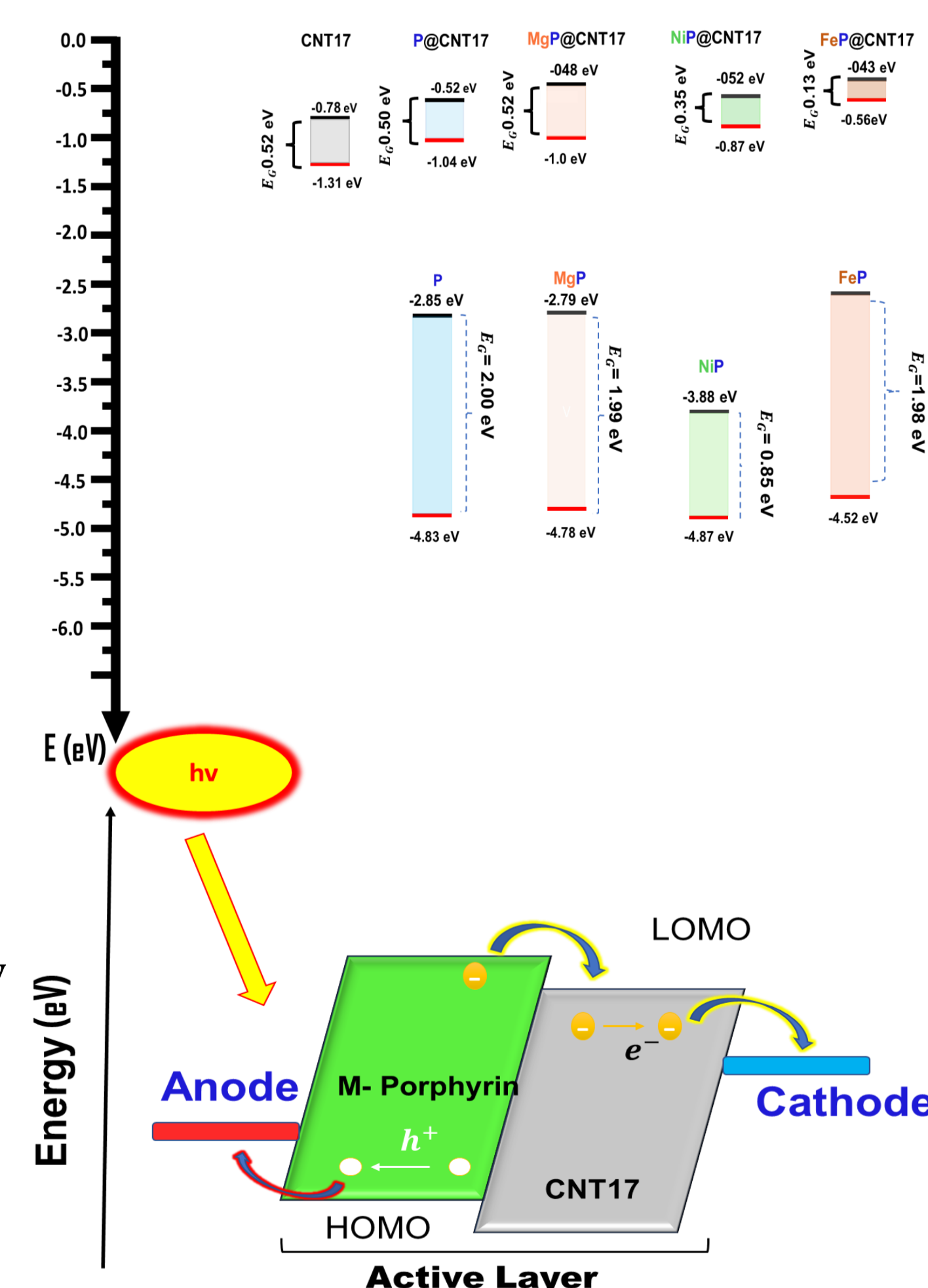
Optical properties

- The optical absorption edges of the encapsulated systems are slightly shifted to higher energy levels compared to the isolated SWNT17.
- The stability of the hybrids under the UV-visible spectrum.



Conclusion

- Bandgap Reduction:** Encapsulation of NiP, FeP and other Metalloporphyrin in SWNT17 reduces the bandgap, promoting effective charge separation in OSCs.
- Charge Transfer:** Encapsulation enhances charge transfer from NiP and FeP to SWNT17, crucial for improving device efficiency.
- Optical Absorption:** NiP and FeP molecules exhibit strong optical absorption in the visible light region, ideal for OSC active layers.
- Light Trapping:** Hybrid structures show reduced reflectance, improving light trapping, with FeP@SWNT17 having higher reflectance in the visible region.



Perspectives

- Computation of the PCE.
- explore the encapsulation of other molecules, beyond porphyrins, within carbon nanotube.

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References

- [1] Gao, Pingqi, et al. *Advanced science* 5.3 (2018): 1700547.
- [2] Park, Jong Min, et al. *Coordination Chemistry Reviews* 407 (2020): 213157.
- [3] Shuixing Li, et al. *Advanced Materials* 2018, 30 (6), 1705208.
- [4] N Thovhogi, et al. *Proceedings* 2015, 2 (7), 4053-4059.
- [5] Georg Kresse, et al. *Physical review B* 1996,54 (16), 11169.