Assessing the Synthetic Compatibility of GDB-9 Molecules with PCBM and PCDTBT for Organic Solar Cells

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Context and Motivation

Diagrammatic representation of various properties of organic materials

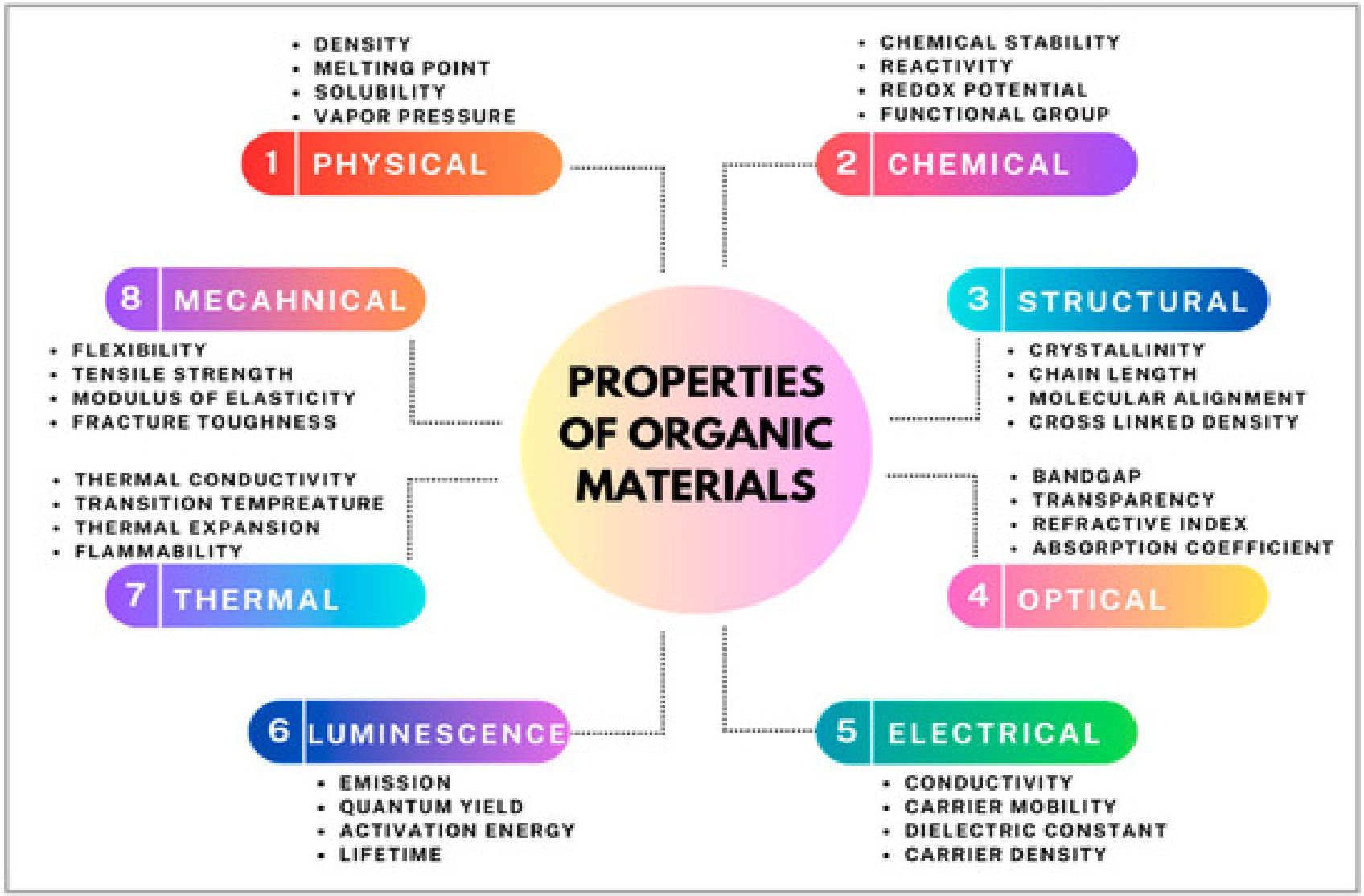

Figure 1: https://doi.org/10.3390/org5040028.

Context and Motivation

Linking Molecular Innovation to Energy, Health, and Display Technologies

Solar Energy Sector

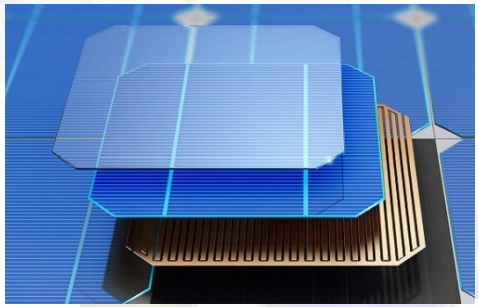

Figure 2: *Organic photovoltaic cells (OPVs) for next-gen solar panels.*

Pharmaceutical Industry

Figure 3: *Bioactive molecules for drug discovery and delivery.*

Organic Electronics

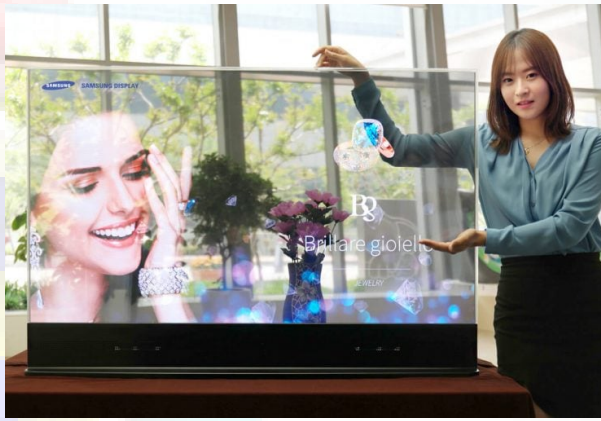

Figure 4: *OLED displays and sensors using advanced fluorophores.*

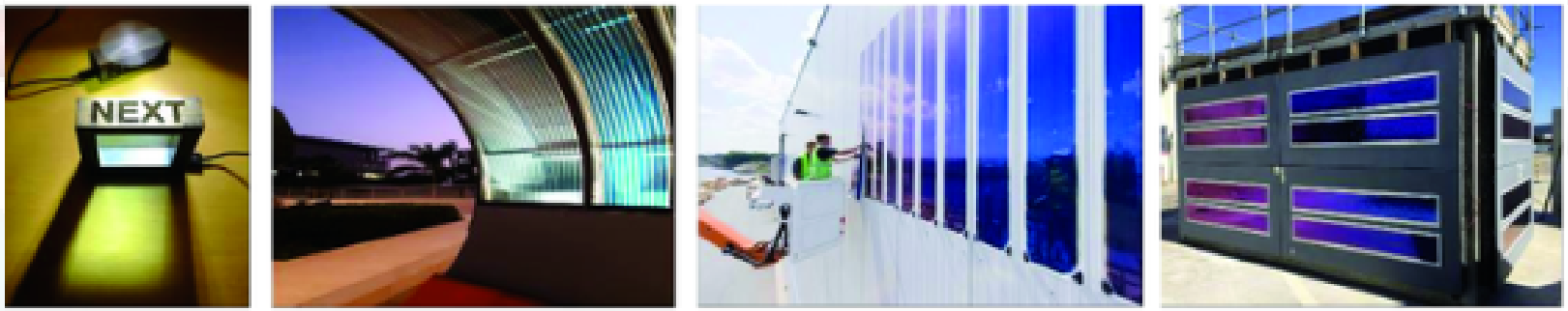

Figure 5: *Versatile application scope of organic materials: OPV, OLED, and beyond.*

Acceptor (PCBM):

- Fullerene structure (C_{60}): 60 carbon atoms
- Low LUMO level facilitating electron injection
- High chemical and thermodynamic stability

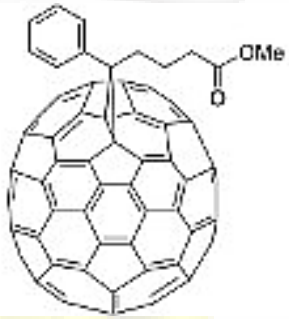

Figure 6: *$PC_{60}BM$*

1. **PCBM: 6.5% efficiency**
2. **PCDTBT: 7.2% efficiency**
3. **PCBM-PCDTBT blend: 9% efficiency**

Donor (PCDTBT):

- Thiophene groups for enhanced electronic conjugation
- High HOMO level favoring electron donation
- High solubility for active layer film fabrication

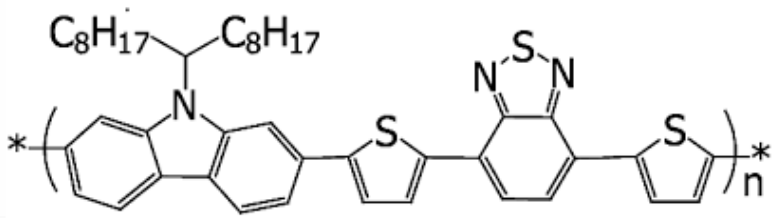

Figure 7: *PCDTBT*

References: He, Y., et al., Advanced Materials (2004); Li, G., et al., Nature Photonics (2010); Zhao, J., et al., Chemical Reviews.

Context and Motivation

Emerging Organic Materials for Sustainable Photovoltaics (SDG 7 and 13)

Cell Type	$ Cost ($/W)	Form Factor	Advantages	CO_2 (g/kWh)
Homojunction Silicon	15–20	Rigid	High durability, mature tech	40–70
Heterojunction Silicon	20–25	Thin rigid (¡120µm)	Higher efficiency, thinner	40–60
Homojunction OPV	5–10	Flexible	Low-cost, printable, lightweight	20–40
Heterojunction OPV	8–12	Flexible	Customizable, low energy cost	20–50
Perovskite	10–15	Rigid or flexible	High efficiency, emerging tech	35–80

Table 1: ***Comparative metrics for photovoltaic technologies (NREL, IEA, Fraunhofer, 2024)***

- Organic photovoltaics (OPVs) offer flexibility, tunability, and scalable production — ideal for off-grid and wearable technologies.
- However, their PCE is still limited by molecular-level challenges: stability, charge transport, and exciton dissociation.

Contents

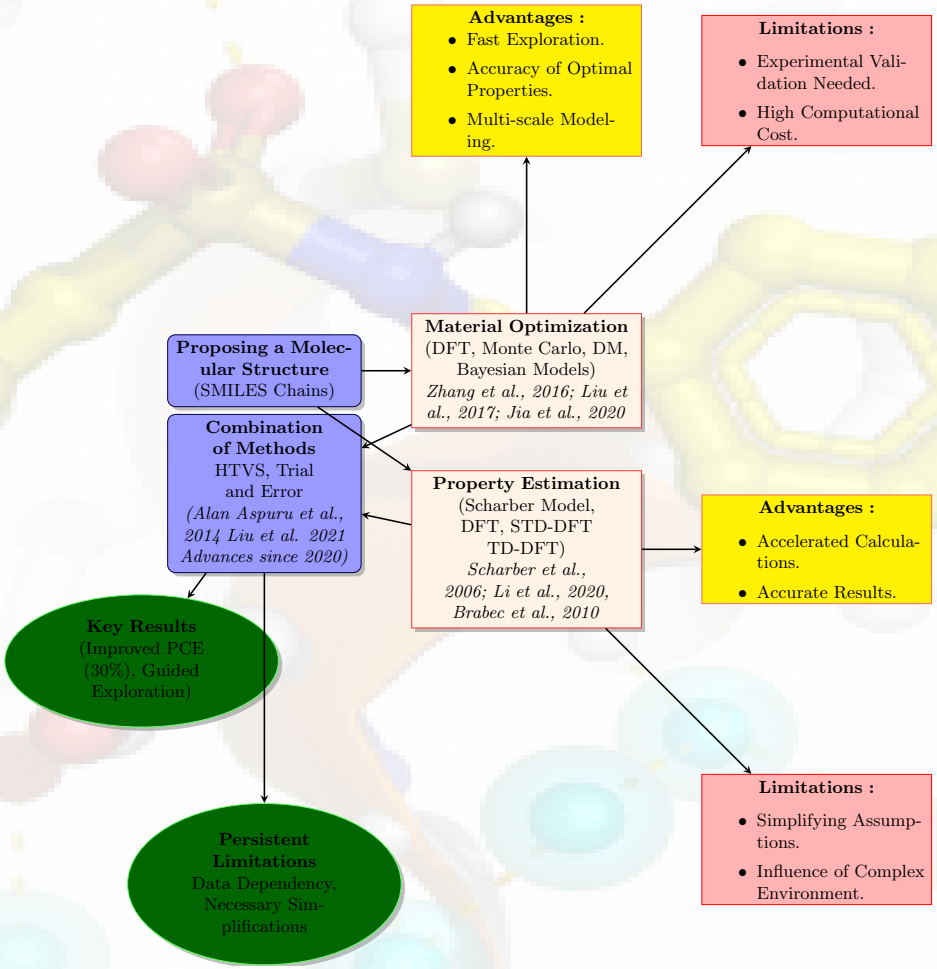

Figure 8: *Integrated Approaches for the Design, Optimization approaches for synthesis of Organic Materials*

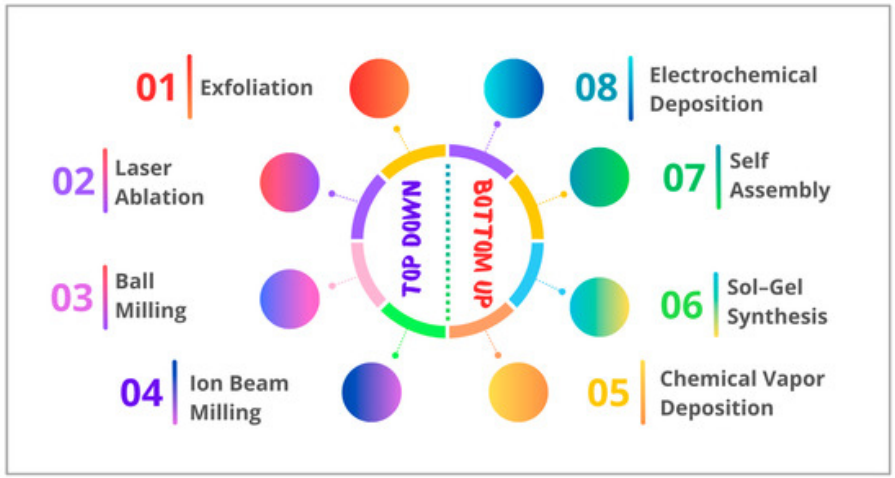

Figure 9: *Diagrammatic representation of top-down and bottom-up approaches for synthesis of organic materials*

Literature Review

Process flow diagram of key stages of the review

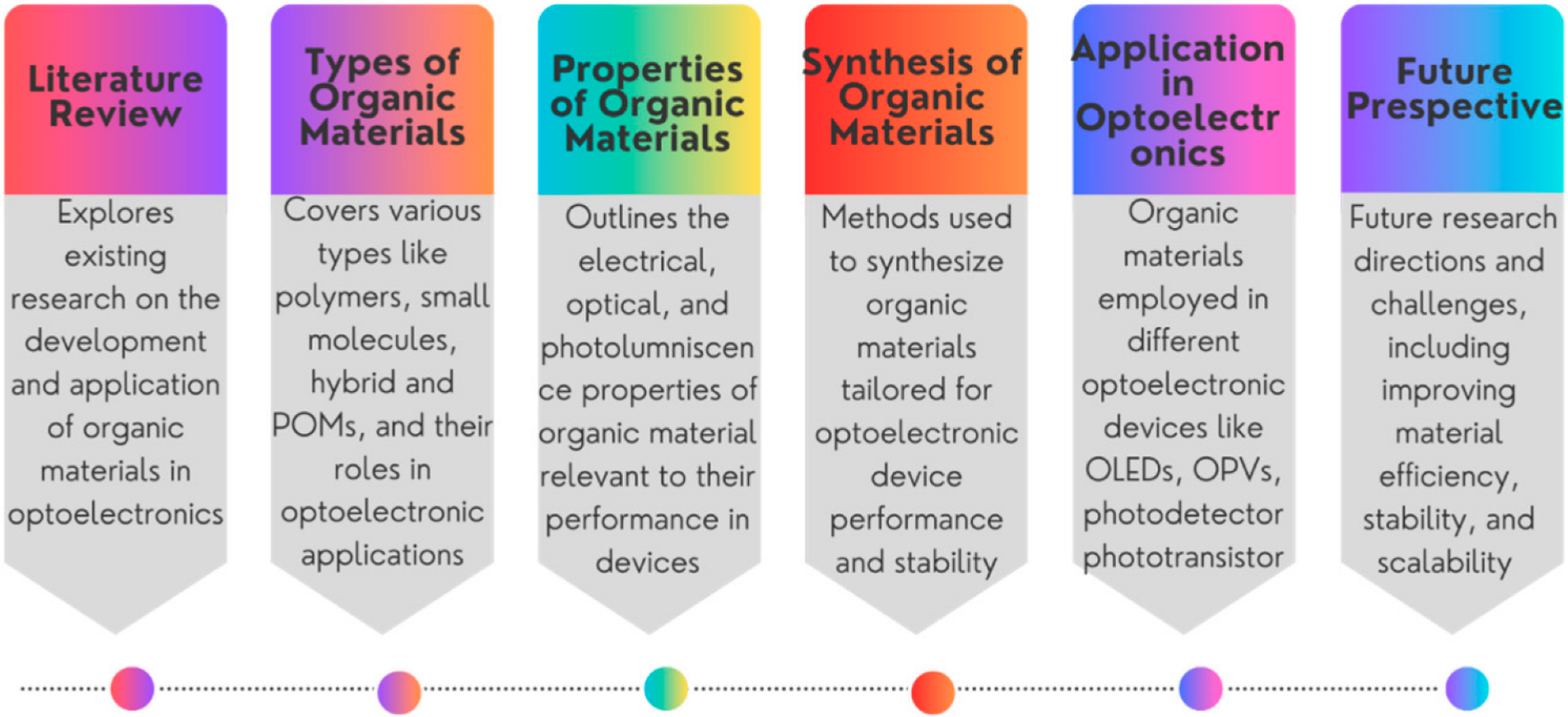

Figure 10: *.https://doi.org/10.3390/org5040028*

Why GDB9?

Thousands of synthetically diverse small molecules with rich chemical diversity — but not all are OPV-compatible or synthetically accessible.

Context (EN)

- **GDB9 database** : Theoretical small molecules, limited synthetic realism
- **Main challenge** : Identify OPV-compatible molecules with poor synthetic accessibility
- **Extended question** : Could these molecules serve other purposes?

Key Case: BODIPY

- Strong fluorescence, tunable scaffold
- Applications: OPV, OLEDs, biosensors, medical imaging

Strategy:

From computational screening to experimental synthesis — toward cross-domain applications.

Research Problem

Despite promising theoretical performance, many small molecules identified via optoelectronic calculations (DFT, xTB) exhibit poor synthetic accessibility (high SA score), limiting their experimental transferability.

Research Question

How can we identify, among GDB9-derived molecules, those that are not only compatible with OPV materials (PCBM and PCDTBT) but also potentially applicable to other fields such as OLEDs or medicine?

Hypothesis

A strategy combining computational screening, synthetic feasibility evaluation, and exploration of secondary properties enables the identification of versatile molecules suitable for multiple technologies.

General Objective

To design small organic molecules derived from GDB9 with high potential for OPV, while assessing their cross-domain applicability (e.g., TADF materials, bioimaging agents) through a structured computational workflow.

Specific Objectives

1. Optimize molecular structures (xTB, CREST) and extract key electronic properties (HOMO, LUMO, gap).
2. Estimate photovoltaic efficiency (PCE) using the Scharber model.
3. Identify donor molecules compatible with PCBM and acceptors compatible with PCDTBT.
4. Filter molecules based on their SA score (synthetic feasibility).
5. Explore alternative applications via secondary properties (fluorescence energy, triplet gap, QED...).

Scharber Model

Developed by Mark Scharber et al. in 2010, this physical model is used to describe the behavior of organic photovoltaic (OPV) cells.

Power Conversion Efficiency (PCE)

This metric evaluates the performance of the photovoltaic cell:

$$\text{PCE} = 100 \cdot \frac{V_{oc} \cdot FF \cdot J_{sc}}{P_{in}}. \quad (1)$$

$$J_{sc} = A \cdot e^{-E_{GAP}^2/B}. \quad (2)$$

$$V_{oc} = \frac{1}{e}\left(|E_{HOMO}^{Do}| - |E_{LUMO}^{Ac}| - 0.3\right). \quad (3)$$

- V_{oc}: Open-circuit voltage in V.
- FF: Fill factor (in %).
- J_{sc}: Short-circuit current density in A/m^2.
- P_{in}: Incident light intensity in W/m^2.
- A, B: Fitting parameters.

Synthetic Accessibility and OPV Compatibility

- The **Synthetic Accessibility Score (SA)** evaluates molecular synthesizability on a scale from 1 (easy) to 10 (hard).
- To select efficient and feasible candidates, we define: $PCE_{SAS} = PCE - SAs$
- High PCE_{SAS} values indicate strong photovoltaic potential and practical synthesis feasibility.

Toward Multifunctionality TADF

- **Singlet–Triplet Gap** $\Rightarrow$ used to predict TADF potential in OLEDs.
- **Radiative Lifetime (τ)** computed as: $\tau = \frac{c^3}{2 \cdot E_f^2 \cdot f} \cdot t_{au}$

  where E_f = fluorescence energy, f = oscillator strength, t_{au} = time conversion factor.
- **Multi-Objective Function:**

$$\text{Multi\_Obj} = f - \Delta E_{ST} - |E_f - 3.2|$$

  Encourages: strong oscillator strength, low singlet–triplet gap, and fluorescence near 3.2 eV.
- **Physicochemical properties** (QED, LogP, AlogP, HBA, HBD, TPSA, CX LogD) are explored for biomedical or diagnostic applications.

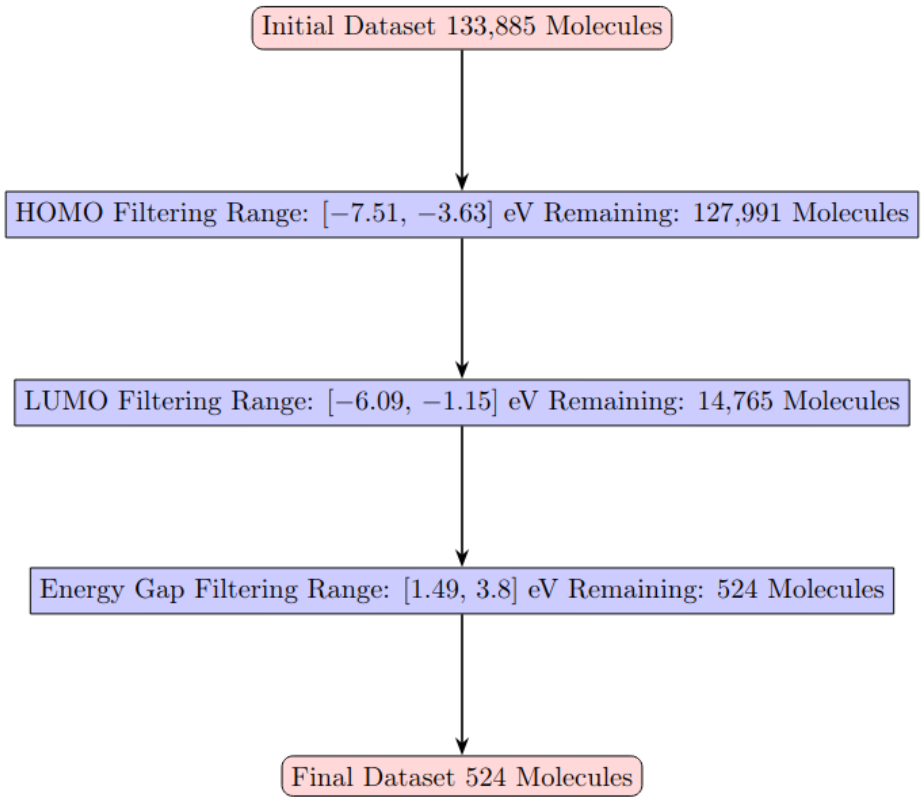

Figure 11: *Stepwise filtering process of the initial molecular dataset using HOMO, LUMO, and energy gap thresholds. The final subset comprises 524 molecules suitable for OPV applications.*

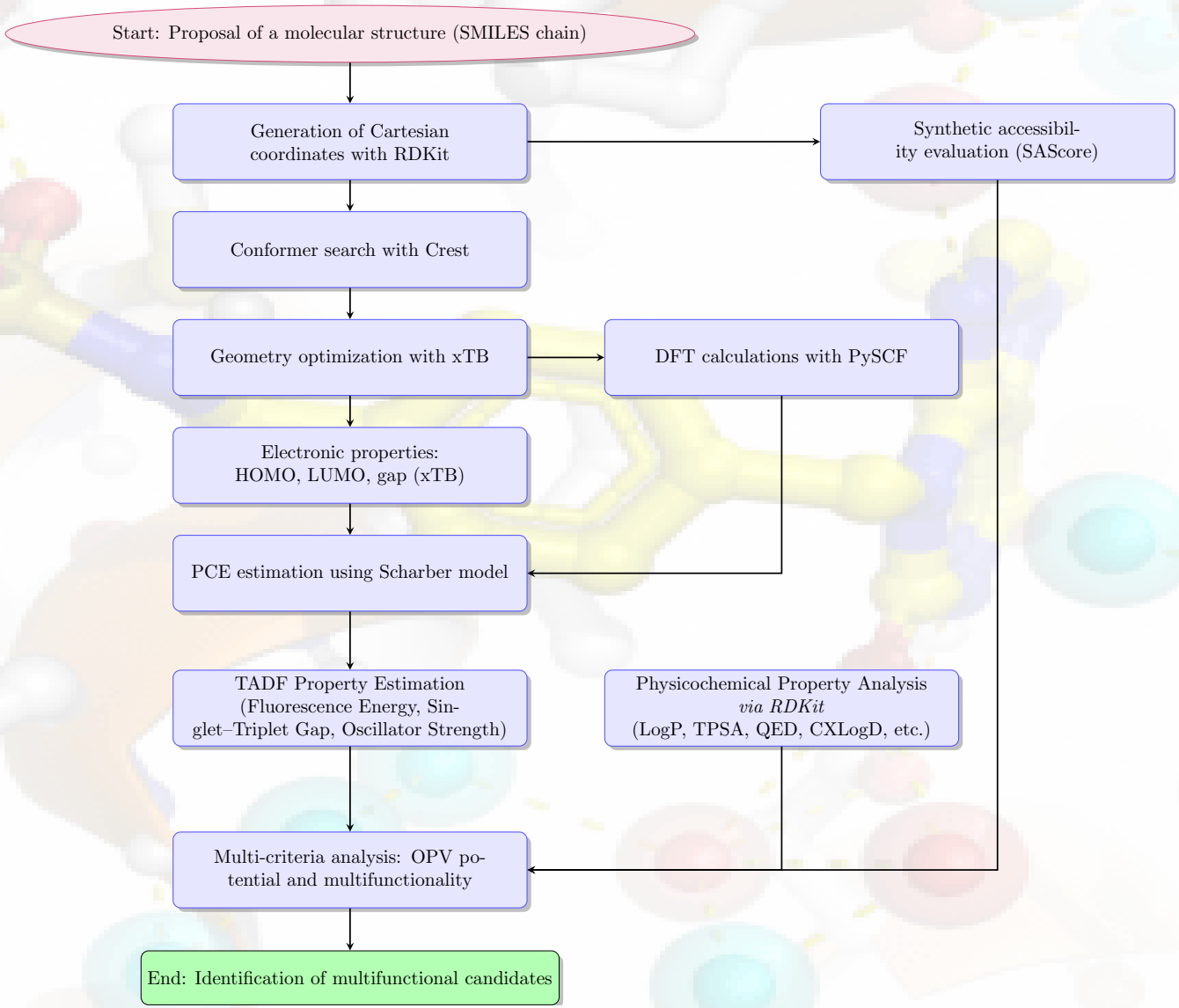

Figure 12: *Complete workflow for OPV optimization.*

Results and Discussion

Molecular Optimization and Electronic Properties

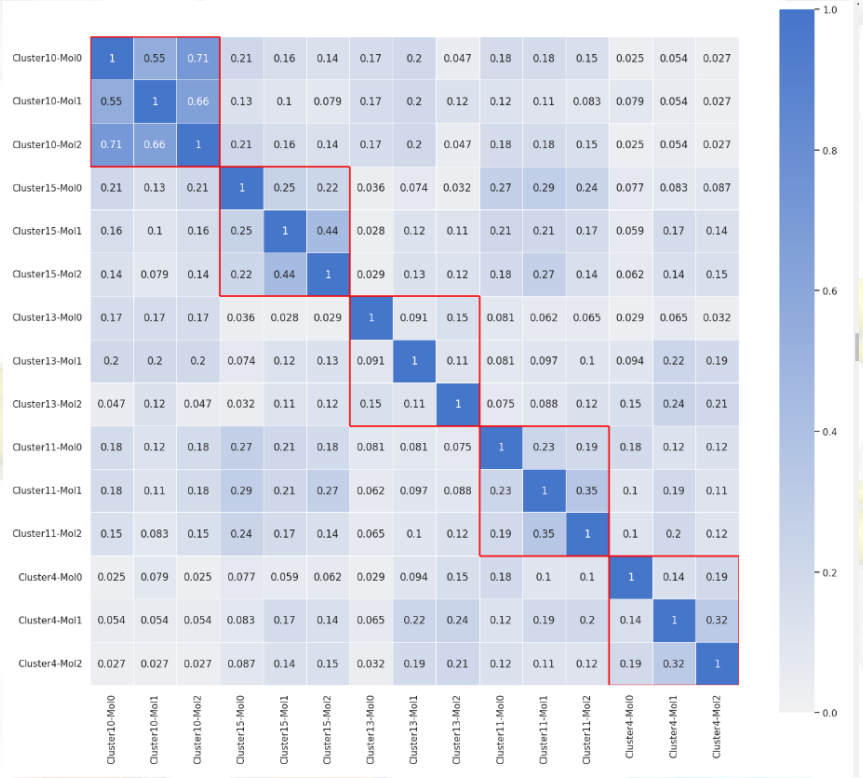

Figure 13: *Tanimoto similarity matrix between molecules in clusters including the reference compounds (Mol0) and three test compounds (Mol1, Mol2, Mol3).*

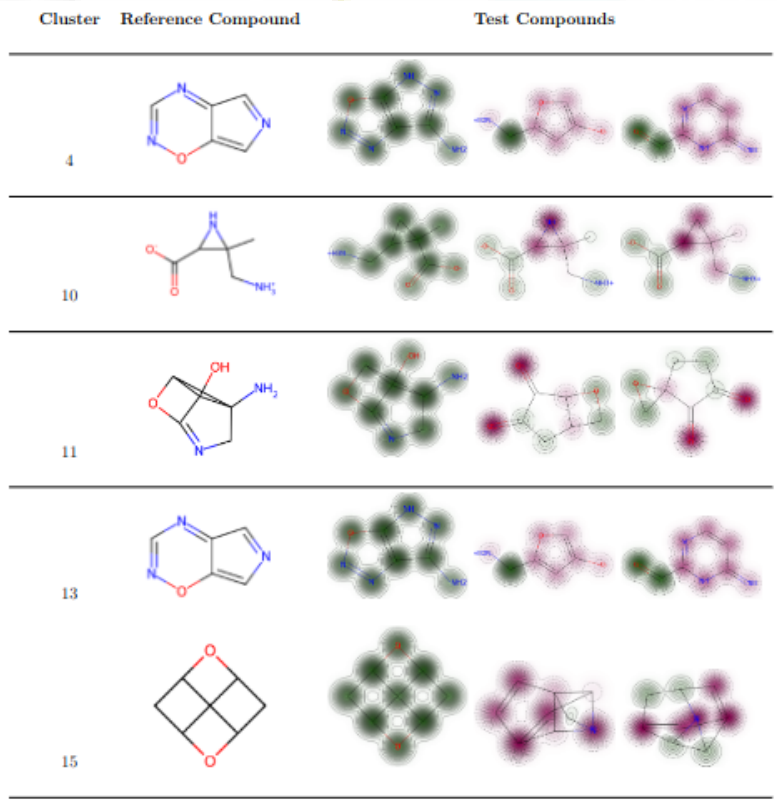

Figure 14: *The similarity weights were visualized by colors on the structure (similarity maps). Sub- structures that increase the similarity score were presented in green, whereas red indicates the opposite.*

Results and Discussion

Molecular Optimization and Electronic Properties: GFN-xTB MAE values

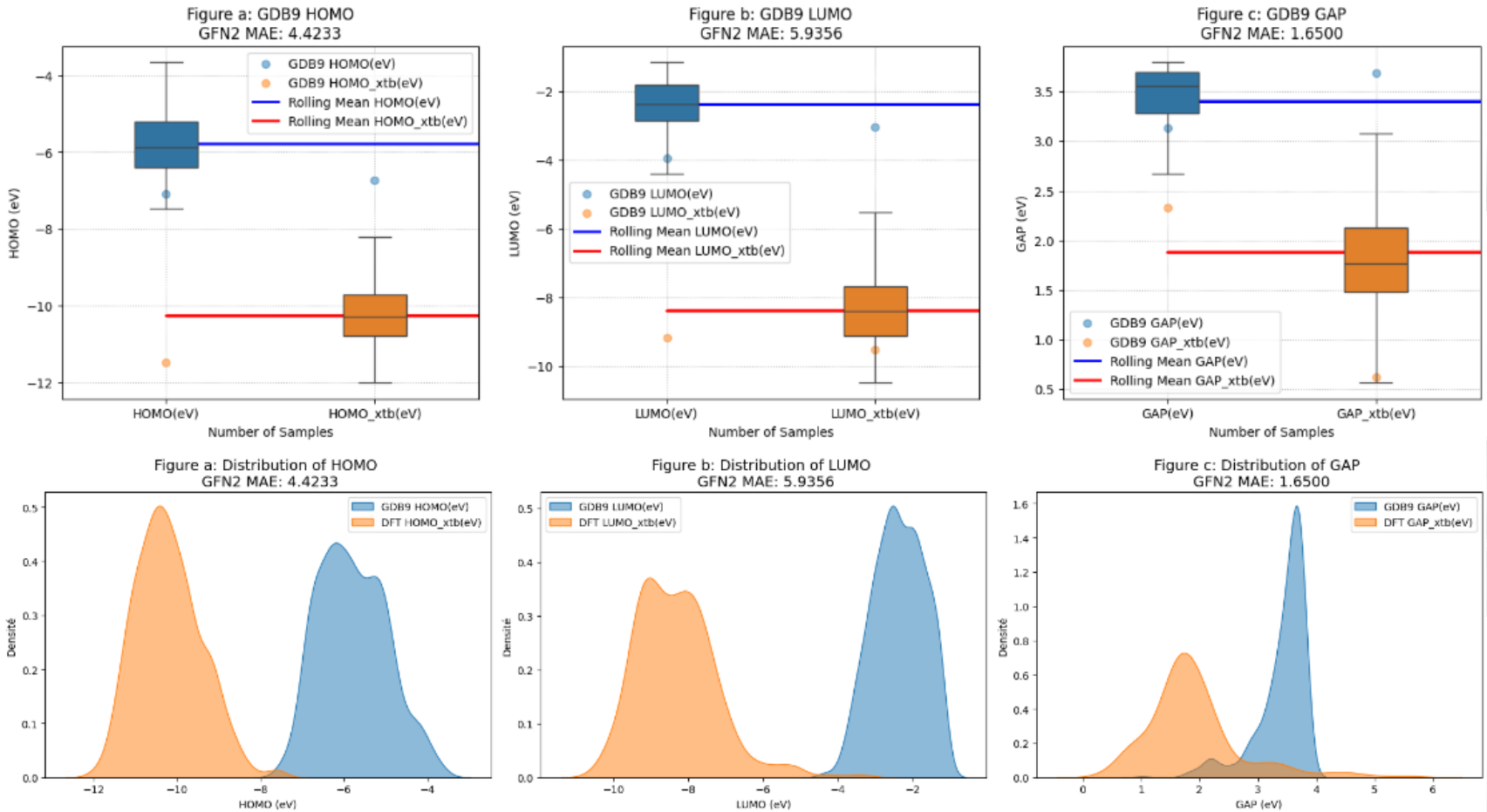

Figure 15: *HOMO, LUMO, and GAP distributions with GFN2 MAE values*

Results and Discussion

Molecular Optimization and Electronic Properties: RMSD distributions from optimization with GFN-xTB

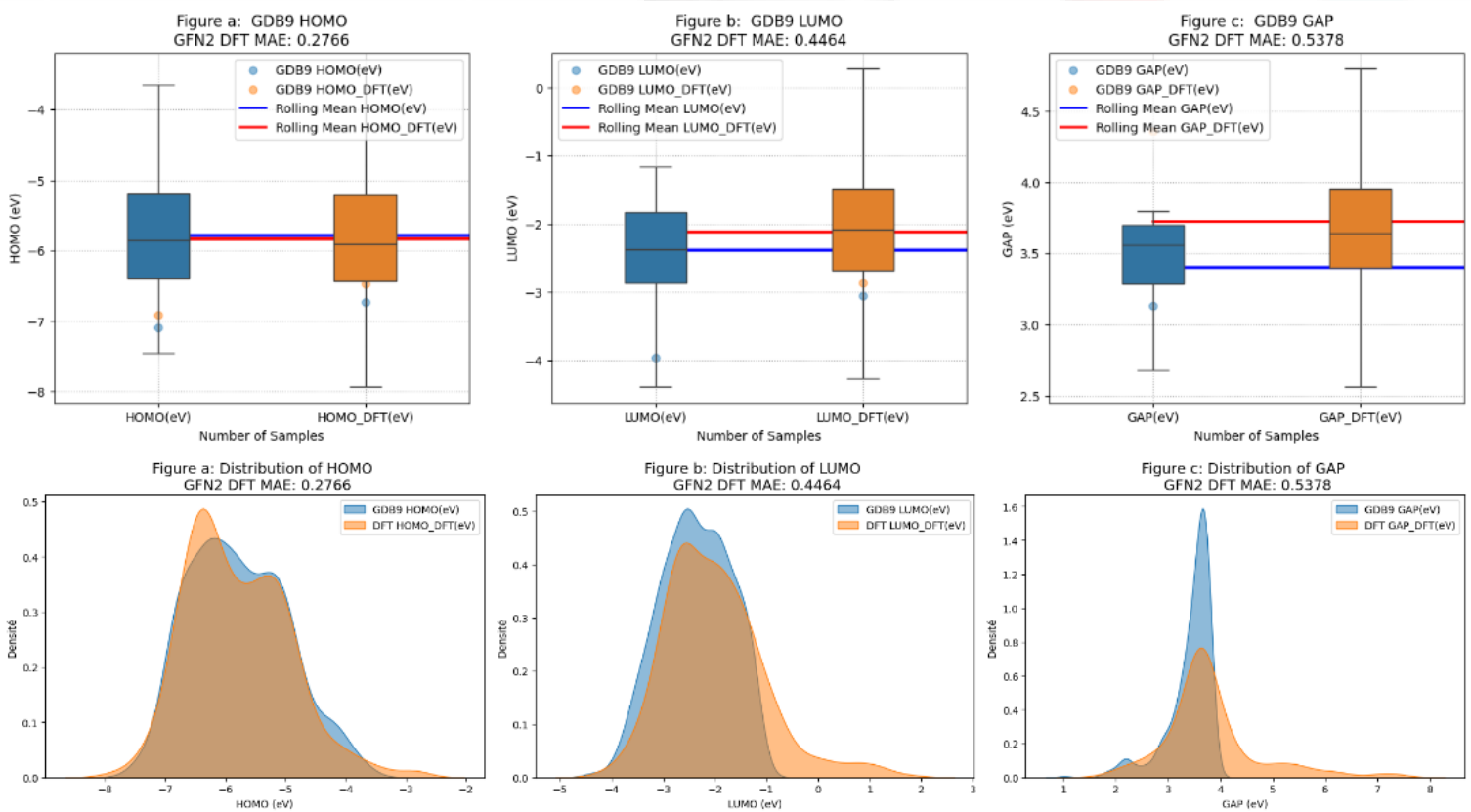

Figure 16: *HOMO, LUMO, and GAP distributions with GFN2-DFT MAE values.*

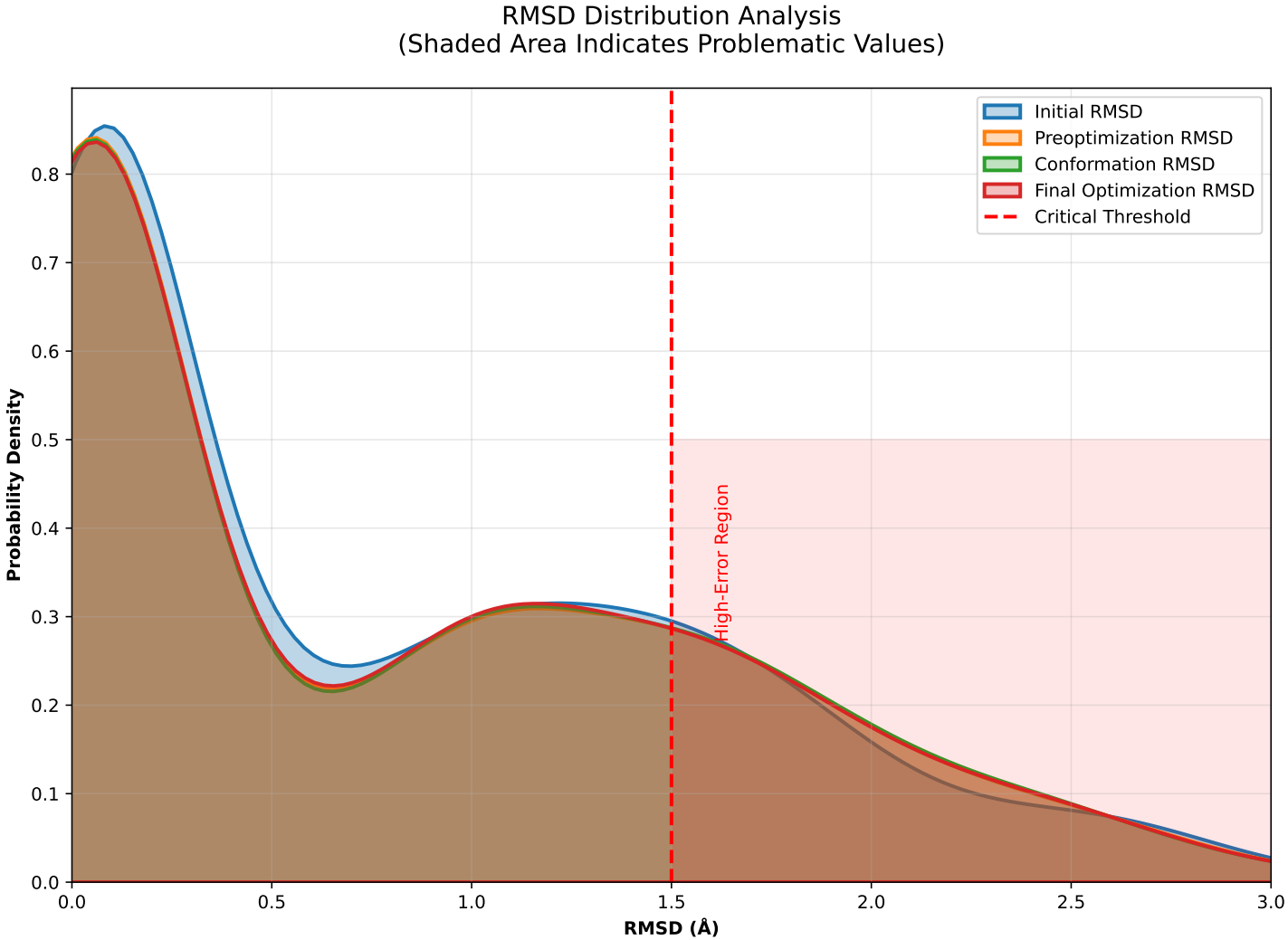

Figure 17: *RMSD distributions from optimization with GFN2.*

Results and Discussion

PCE and SAScore Results

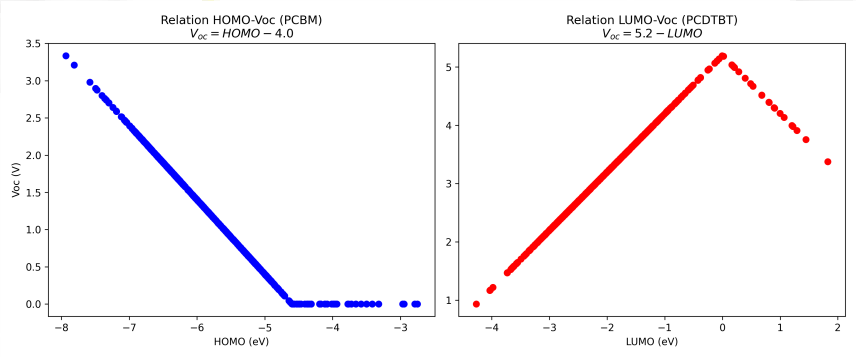

Figure 18: *VOC PCBM distributions from optimization with GFN2.*

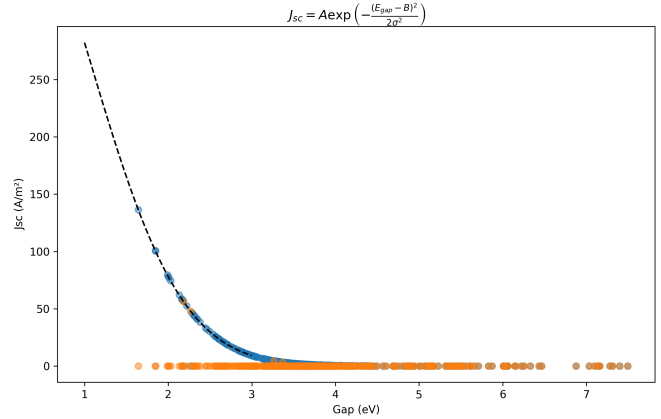

Figure 19: *PCE SAscore GDB9 and HCE distributions from optimization with GFN2 .*

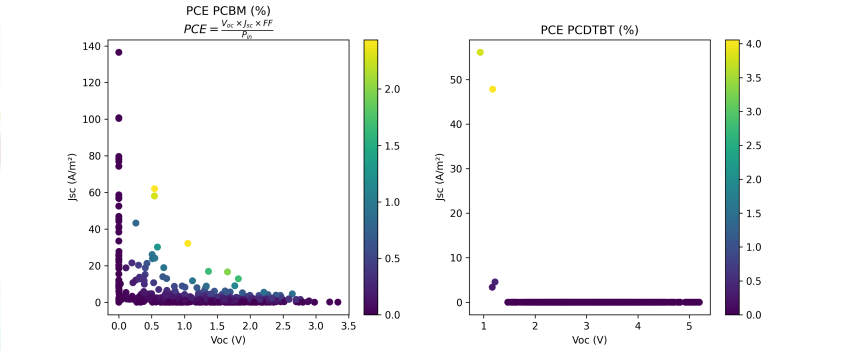

Figure 20: *PCE contribution from optimization with GFN2.*

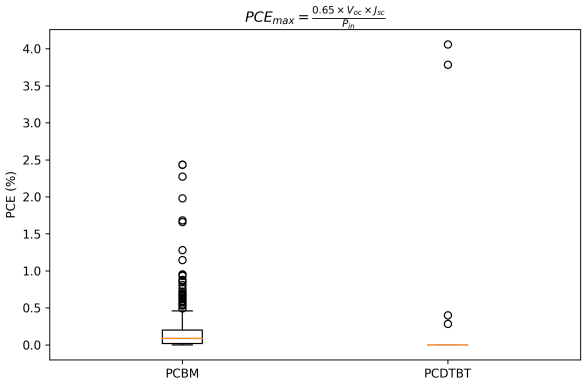

Figure 21: *PCE GDB9 and HCE distributions*

Results and Discussion

PCE and SAScore Results

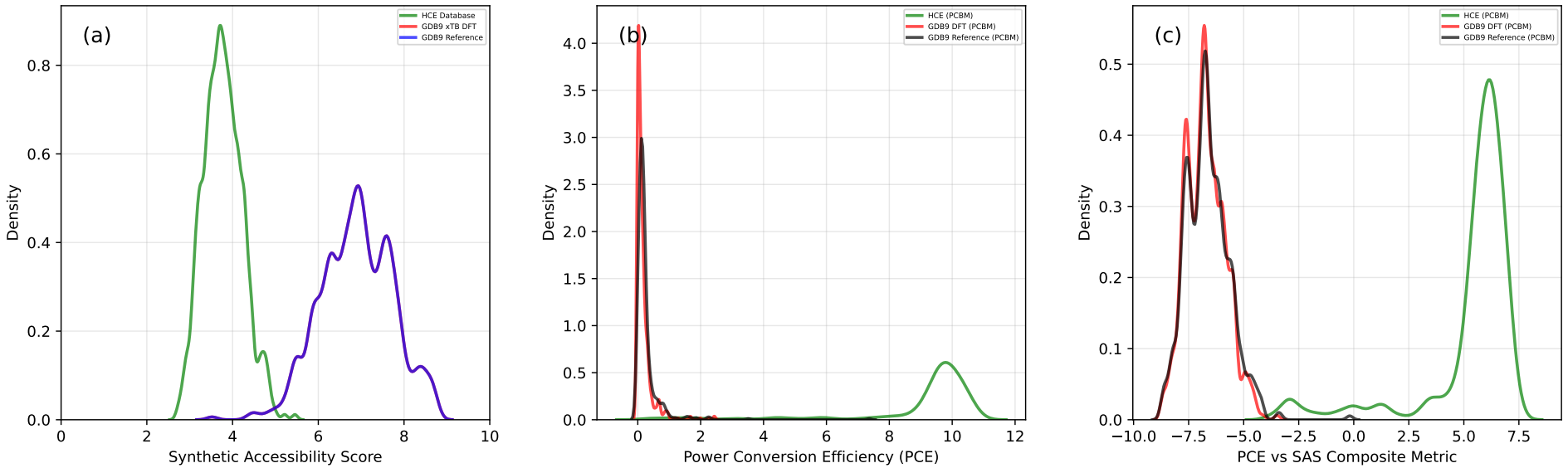

Figure 22: *Comparative analysis of molecular databases: (a) Synthetic accessibility score (SAS) distributions showing HCE database, GDB9 xTB DFT, and reference GDB9 data; (b) Power conversion efficiency (PCE) distributions for PCBM-based systems; (c) Composite metric analyzing PCE-SAS relationship. All density estimates calculated with Gaussian KDE (bandwidth = 0.5).*

Molécule	pIC_{50}	IC_{50} (nM)	MW	LogP	AlogP	HBA	HBD	TPSA	QED	CX LogD	CSP3	Rings
D_43243	8.34	4.57	119.12	0.08	0.08	1	0	20.08	0.413	0.08	0.29	3
D/A_21398	8.34	4.55	109.09	-1.25	-1.25	5	1	75.41	0.451	-1.25	0.00	1
A_8723	8.36	4.39	114.06	-1.48	-1.48	4	0	68.28	0.255	-1.48	0.00	0

Table 2: ***Key descriptors of selected GDB-9 donor and acceptor candidates.*** *Physicochemical and bioactivity properties relevant to organic photovoltaic (OPV) compatibility with PCBM and PCDTBT.*

Table 3: ***Photophysical and quantum chemical descriptors of selected GDB-9 molecules.*** *Key properties such as fluorescence energy, singlet–triplet gap, oscillator strength, and computed lifetimes are summarized for a selection of molecules from the GDB-9 dataset. These results stem from DFT and TDDFT calculations and may inform future material design in optoelectronics and biomedical applications.*

Molecule	Fluorescence Energy (eV)	Singlet–Triplet Gap (eV)	Oscillator Strength	Lifetime (ns)	Multi-Obj
D_43243	3.561	1.597	0.0191	95.02	-1.938
D/A_21398	0.914	0.632	0.0011	24314.55	-2.917
D_8723	2.625	0.510	0.0003	11252.30	-1.085

General Conclusion and Outlook

Conclusion

- Molecules `D_43243`, `D/A_21398`, and `A_8723` show promising balance between OPV efficiency and synthetic accessibility.
- Their photophysical features (low E_{ST}, fluorescence) and biochemical properties (LogP, QED) point to multifunctional potential.
- The PCE_{SAS} score proves useful in identifying practical and efficient candidates from a wide chemical space.

Perspectives

- **OPV:** Experimentally validate molecules with high PCE_{SAS} and favorable electronic profiles.
- **OLEDs:** Investigate TADF potential via singlet–triplet gap and lifetime analysis.
- **Biomedical:** Explore bioactivity for applications in molecular imaging or therapeutic targeting.


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