High-Throughput Virtual Screening of Existing Organic Chromophores for Materials Discovery

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Abstract

High-throughput virtual screening (HTVS) has emerged as a powerful tool for organic electronics discovery, driven by advancements in hardware, computational methods, and access to extensive experimental and theoretical datasets. We have leveraged HTVS[1] using the Cambridge Structural Database[2] to identify candidates for singlet fission,[3,4] thermally activated delayed fluorescence,[5] non-fullerene electron acceptors,[6] and luminescent crystals with superradiance or near-infrared emission.[7] Screening experimentally verified structures enables the identification of real, synthetically-accessible candidates, avoiding the major limitation of de novo studies.

Our latest HTVS study extends to the much larger ZINC database,[8] comprising millions of commercially available organic compounds. Using conjugated core clustering, conformational analysis, experimental calibration, and rigorous benchmarking, we assessed the electronic structures of approximately 13 million molecules via TD-DFT, computing around 150,000 unique structures—one of the largest quantum chemical datasets to date. This approach has led to the identification and experimental verification of materials exhibiting near-infrared and anti-Kasha dual emission, with implications for advanced photonic devices.

A particularly intriguing phenomenon emerging from our dataset is the violation of Hund's rule in certain molecules, where an inverted singlet-triplet gap[9] arises due to atom-localized intramolecular charge transfer and spin polarization. This design principle, identified with high-level multireference wavefunction methods, offers new opportunities for OLEDs and other devices requiring efficient triplet harvesting.

Additionally, recent work[10] has evaluated the effectiveness of fine-tuning GPT-3 for predicting electronic and functional properties of organic molecules. The findings suggest that fine-tuned GPT-3 can successfully identify and distinguish chemically meaningful patterns, exhibiting robust predictive performance.

References

[1] Ö. H. Omar, T. Nematiaram, A. Troisi, and D. Padula, Sci. Data, 9 (2022) 54.

[2] C. R. Groom, I. J. Bruno, M. P. Lightfoot, and S. C. Ward, Acta Crystallogr. Sect. B Struct. Sci. Cryst. Eng. Mater., 72 (2016) 171–179.

[3] D. Padula, Ö. H. Omar, T. Nematiaram, and A. Troisi, Energy Environ. Sci., 12 (2019) 2412–2416.

[4] Ö. H. Omar, D. Padula, and A. Troisi, ChemPhotoChem, 4 (2020) 5223–5229.

[5] K. Zhao, Ö. H. Omar, T. Nematiaram, D. Padula, and A. Troisi, J. Mater. Chem. C, 9 (2021) 3324–3333.

[6] Z. W. Zhao, Ö. H. Omar, D. Padula, Y. Geng, and A. Troisi, J. Phys. Chem. Lett., 12 (2021) 5009–5015.

[7] T. Nematiaram, D. Padula, and A. Troisi, Chem. Mater., 33 (2021) 3368–3378.

[8] J. J. Irwin and B. K. Shoichet, J. Chem. Inf. Model., 45 (2005) 177–182.

[9] P. De Silva, J. Phys. Chem. Lett., 10 (2019) 5674–5679.

[10] Z. Xie, X. Evangelopoulos, Ö. H. Omar, A. Troisi, A. I. Cooper, and L. Chen, Chem. Sci., 15 (2024) 500–510.