

## **Non-covalent interactions (NCIs) in $\pi$ -conjugated functional materials: Advances and perspectives**

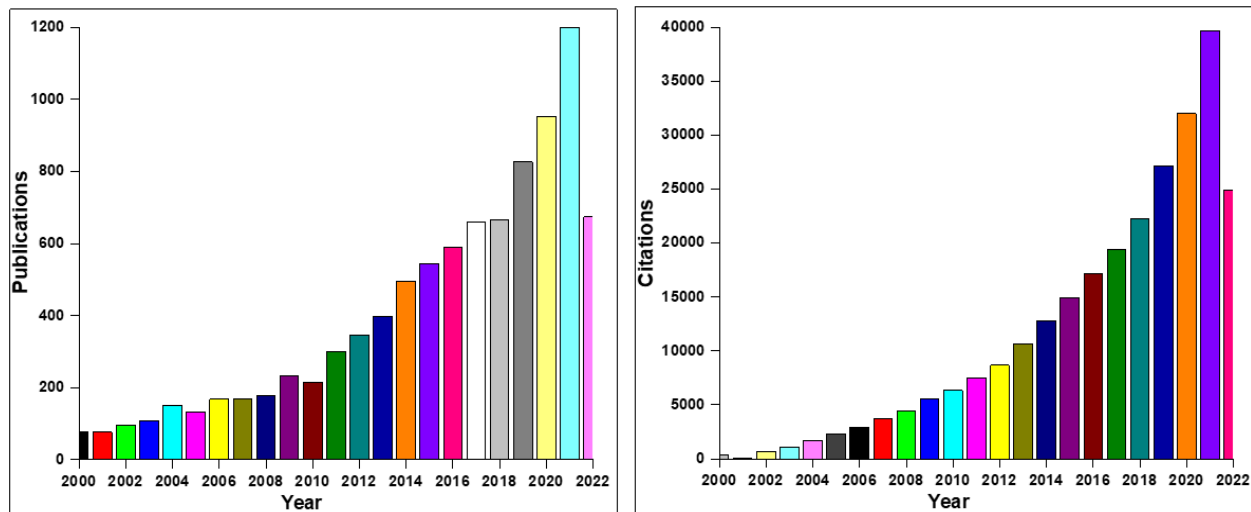
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**Fig. S1:** Histogram showing the number of publications and citations on the topic “*non-covalent interactions*”. (Data searched from Web of Science on September 2, 2022. These materials are reproduced under a license from Thomson Reuters. You may not copy or re-distribute these materials in whole or in part without the prior written consent of Thomson Reuters).

**Table T1:** Intermolecular interactions characterization techniques in  $\pi$ -conjugated materials.

Experimental techniques	NCI studied	References
IR/Raman	Hydrogen bonding, Metal coordination	1, 2, 3
NMR	Hydrogen bonding	1, 2
NEXAFS	Metal insertion	3
AFM	Hydrogen bonding, van der Waals interactions, host-guest interactions, cation- $\pi$ interactions	4-10
STM	Short-range Pauli repulsion, van der Waals forces, electrostatic repulsions, and halogen bonds	11-13
Kelvin probe force microscopy (KPFM)	$\sigma$ -hole interactions	14, 15
3D Electron Diffraction	Multiple NCIs	16
DFM	H-bonding	9

### References

1. M. U. Ocheje, B. P. Charron, Y.-H. Cheng, C.-H. Chuang, A. Soldera, Y.-C. Chiu and S. Rondeau-Gagné, *Macromolecules*, 2018, **51**, 1336-1344.
2. J. Yao, C. Yu, Z. Liu, H. Luo, Y. Yang, G. Zhang and D. Zhang, *J. Am. Chem. Soc.*, 2016, **138**, 173-185.
3. K. Bae, D. G. Lee, M. I. Khazi and J. M. Kim, *Macromolecules*, 2022, **55**, 2882-2891.
4. H. Mönig, S. Amirjalayer, A. Timmer, Z. Hu, L. Liu, O. Díaz Arado, M. Cnudde, C. A. Strassert, W. Ji and M. Rohlfing, *Nature Nanotechnology*, 2018, **13**, 371-375.
5. J. Zhang, P. Chen, B. Yuan, W. Ji, Z. Cheng and X. Qiu, *Science*, 2013, **342**, 611-614.
6. J. Nie, Y. Deng, F. Tian, S. Shi and P. Zheng, *Nano research*, 2022, **15**, 4251-4257.
7. C.-I. Chiang, C. Xu, Z. Han and W. Ho, *Science*, 2014, **344**, 885-888.
8. L. Gross, F. Mohn, N. Moll, P. Liljeroth and G. Meyer, *Science*, 2009, **325**, 1110-1114.
9. A. Sweetman, S. P. Jarvis, H. Sang, I. Lekkas, P. Rahe, Y. Wang, J. Wang, N. R. Champness, L. Kantorovich and P. Moriarty, *Nature Communications*, 2014, **5**, 1-7.
10. S. Kawai, A. S. Foster, T. Björkman, S. Nowakowska, J. Björk, F. F. Canova, L. H. Gade, T. A. Jung and E. Meyer, *Nature communications*, 2016, **7**, 1-7.
11. G. Kichin, C. Weiss, C. Wagner, F. S. Tautz and R. Temirov, *J. Am. Chem. Soc.*, 2011, **133**, 16847-16851.
12. Z. Han, G. Czap, C.-I. Chiang, C. Xu, P. J. Wagner, X. Wei, Y. Zhang, R. Wu and W. Ho, *Science*, 2017, **358**, 206-210.
13. J. Lawrence, G. C. Sosso, L. Đorđević, H. Pinfold, D. Bonifazi and G. Costantini, *Nature communications*, 2020, **11**, 1-7.
14. F. Mohn, B. Schuler, L. Gross and G. Meyer, *Appl. Phys. Lett.*, 2013, **102**, 073109.
15. B. Mallada, A. Gallardo, M. Lamanec, B. De La Torre, V. Špirko, P. Hobza and P. Jelinek, *Science*, 2021, **374**, 863-867.
16. Y. Luo, M. T. Clabbers, J. Qiao, Z. Yuan, W. Yang and X. Zou, *J. Am. Chem. Soc.*, 2022.