

Studying Organic Solar Cell Materials Using the Condensed to Atoms Fukui Indexes

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In the last two decades, the demand for efficient and sustainable ways of producing electricity increased, motivating the development of high-efficient photovoltaic devices. In this context, bulk heterojunction organic solar cells based on non-fullerene acceptor (NFA) molecules have shown promising performances due to their versatility of synthesis, processing advantages, good stability to sunlight exposition, and high efficiencies (of up to 18%) [1]. In particular, the high chemical versatility of these materials allows the synthesis of a number of distinct NFAs with varied performances, so that theoretical studies are essential to guide the prospection of new optimized compounds. One approach is to study the basic fundamentals at molecular level to better understand and what differentiates the NFA based solar cells from other bulk heterojunction solar cells. There are a myriad of tools to use for this purpose, among them there are the Fukui indexes, a reactivity calculation tool that'd been applied successfully to different organic materials and offers insights beyond just reactivity. In this presentation I'd like to show and explain what are the Fukui indexes, when and how to use them, in the context of the organic solar cell materials. The focus is to highlight its usefulness and clarify how they are calculated computationally.

References

- [1] S. Li, L. Ye, W. Zhao, H. Yan, B. Yang, D. Liu, W. Li, H. Ade, J. Hou, A Wide Band Gap Polymer with a Deep Highest Occupied Molecular Orbital Level Enables 14.2% Efficiency in Polymer Solar Cells, *J. Am. Chem. Soc.* 140 (2018) 7159–7167.