**Influence of End-Capped Engineering on 3-Dimenional Star-Shaped Triphenylamine-Based Donor Materials for Efficient Organic Solar Cells**

Muhammad Adnan, *a\*1* Zobia Irshad, *b1* Riaz Hussain, *c\** Wonjong Lee, *a* Jung Yup Yang, *d\** Jongchul Lim *a\**

*a Graduate School of Energy Science and Technology, Chungnam National University, 34134, Daejeon, Republic of Korea*

*b Department of Chemistry, Chosun University, 61452, Gwangju, Republic of Korea*

*c Department of Chemistry, University of Okara, Okara-56300, Pakistan*

*d Department of Physics, Kunsan National University, Geonbuk, 54150 Republic of Korea*

*1 Muhammad Adnan and Zobia Irshad contributed equally for the first authorship.*

***Corresponding authors****:*

*Muhammad Adnan (Ph.D.)* [*adnan5750@gmail.com*](mailto:adnan5750@gmail.com)*,* [*adnan@cnu.ac.kr*](mailto:adnan@cnu.ac.kr)

*Riaz Hussain (Ph.D.)* [*riazhussain@uo.edu.pk*](mailto:riazhussain@uo.edu.pk)

*Jung Yup Yang (Ph.D.)* [*jungyup.yang@kunsan.ac.kr*](mailto:jungyup.yang@kunsan.ac.kr)

*Jongchul Lim (Ph.D.)* [*jclim@cnu.ac.kr*](mailto:jclim@cnu.ac.kr)

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|  |  |
| Reference | STRO1 |
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| STRO2 | STRO3 |
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| STRO4 | STRO5 |
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| STRO6 | STRO7 |
|  |  |
| STRO8 |  |

**Figure S1**: Chemical structure of STRO (R) along-with eight newly proposed star-shaped molecules (STRO1-STRO8).

**Hole Electrons Overlap Heat Maps**

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| Chart  Description automatically generated  **Reference** |
| **Chart  Description automatically generatedSTRO1** |
| Chart  Description automatically generated  **STRO2** |
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| A picture containing graphical user interface  Description automatically generated  **STRO5** |
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| A picture containing diagram  Description automatically generated  **STRO8** |

**Figure S2**: The hole/electrons overlap heat mapsof STRO (R) along-with eight newly proposed star-shaped molecules (STRO1-STRO8).