QM/MM Study of Static and Dynamic Energetic Disorder in the Emission Layer of an Organic Light-Emitting Diode - DTU Orbit (06/12/2018)

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Static and dynamic energetic disorder in emission layers of organic light-emitting diodes (OLEDs) is investigated through combined molecular dynamics and hybrid quantum mechanics/molecular mechanics (QM/MM) calculations. The analysis is based on a comparison of ensemble and time distributions of site energies of guest and host components in an emission layer. The law of total variance is applied to decompose the total disorder into its static and dynamic contributions. It is found that both contributions are of the same order of magnitude. While the dynamic disorder is not affected by intermolecular interactions, the static disorder for both guests and hosts is determined by the polarity of host molecules. The amount of static disorder affects charge-transport properties and exciton formation pathways, which consequently influence the overall efficiency of an OLED device. The simulations indicate that the amount of static disorder induced by the host should be considered for the optimization of the emission layer.

General information
State: Published
Organisations: Massachusetts Institute of Technology
Contributors: de Silva, P., Voorhis, T. V.
Pages: 1329-1334
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: The Journal of Physical Chemistry Letters
Volume: 9
ISSN (Print): 1948-7185
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.37 SJR 4.667 SNIP 1.595
Web of Science (2017): Impact factor 8.709
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.18 SJR 4.602 SNIP 1.651
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 8.04 SJR 4.143 SNIP 1.758
Web of Science (2015): Impact factor 8.539
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 7 SJR 3.725 SNIP 1.71
Web of Science (2014): Impact factor 7.458
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.61 SJR 3.529 SNIP 1.608
Web of Science (2013): Impact factor 6.687
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 6.3 SJR 3.965 SNIP 1.742
Web of Science (2012): Impact factor 6.585
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.95 SJR 3.283 SNIP 1.613
Web of Science (2011): Impact factor 6.213