

## Unravelling the Nature and the Timescale of the Dielectric Constant for Organic Semiconductors

Selim Sami\*<sup>a</sup>, Riccardo Alessandri<sup>b,c</sup>, Ria Broer<sup>b</sup> and Remco W. A. Havenith<sup>a,b</sup>

<sup>a</sup> Stratingh Institute for Chemistry, University of Groningen, The Netherlands,

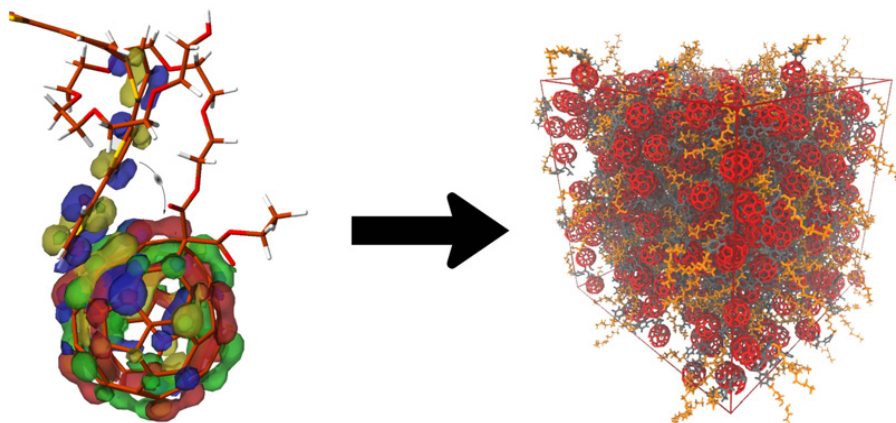
<sup>b</sup> Zernike Institute for Advanced Materials, University of Groningen, The Netherlands,

<sup>c</sup> Groningen Biomolecular Sciences and Biotechnology Institute, University of Groningen, The Netherlands.

s.sami@rug.nl

The current generation of organic photovoltaic devices still lacks the required efficiency to be economically competitive. One way to improve this is to use materials with a high dielectric constant, thereby decreasing the effective coulombic attraction between the electrons and holes and therewith facilitating their transport to the respective electrodes without suffering from recombination [1]. A prominent strategy to this end is the use of ethylene glycol side chains, which are known to increase the dielectric constant drastically [2]. However, both the response timescale and a clear molecular understanding of the origin of the contributions are still lacking.

In this poster, we present a multiscale computational scheme to calculate the different contributions (electronic, dipolar and induced) to the dielectric constant. We employ polarizable force fields for molecular dynamics simulations, for which we derive the parameters from quantum chemical calculations. Having access to detailed molecular information, we are able to decompose the dielectric contributions into molecular fragments, which allows us to clearly pinpoint the origin of these contributions. Moreover, our results, for the first time, unravel the timescale of the contributions and shed light on their relevance for high efficiency organic photovoltaics [3].



### References

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2. F. Jahani, S. Torabi, R.C. Chiechi, L.J.A. Koster, J.C. Hummelen, *Chem. Comm.* **50** (2014) 10645.
3. S. Sami, R. Alessandri, R. Broer, R.W.A. Havenith, in preparation.