The Challenges of Modeling Organic Molecular Materials

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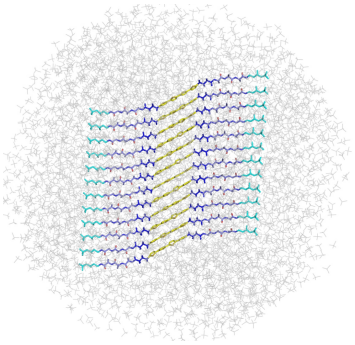
The talk provides an overview of our recent activity, which includes addressing lingering difficulties in describing energies and geometries of systems relevant to the field of organic electronics.[1-5] Emphasis will be placed on DFT[1] and/or SCC-DFTB[2]-based treatments of charged radical oligomers[3] (i.e., charge carrier precursor), charge-transfer interactions,[4] large-scale stacks of oligomers,[3] as well as exciton coupling between polymeric chains.[5]



We will also describe the density-dependent dispersion correction schemes[1] we propose and exploit them to identify the key factors responsible for errors of conventional density functional approximations beyond
van der Waals complexes.

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2. Petraglia, R.; Corminboeuf, C. *J. Chem. Theory Comput.* **2013**, *34*, 2242.
3. Steinmann, S. N.; Corminboeuf, C. *J. Chem. Theory Comput.* **2012,** *8* 4305.
4. Steinmann, S. N.; Piemontesi, C.; Delachat, A.; Corminboeuf, C. *J. Chem. Theory Comput.* **2012***, 8* 1629.
5. Frauenrath, H. *et al*. ACS Nano, **2013**, *7*, 8498.