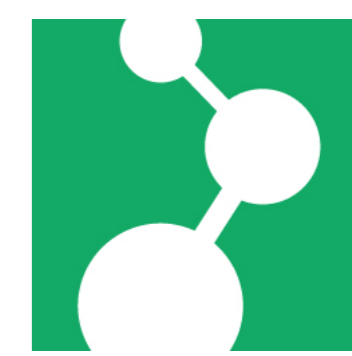




Multiscale approach for organic electronics



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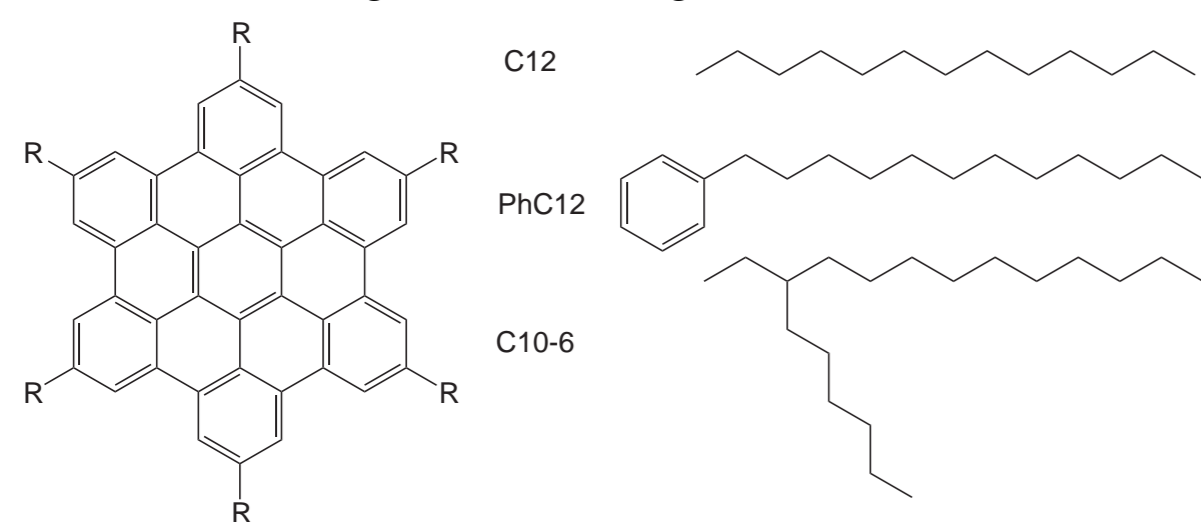
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Atomistic MD simulations

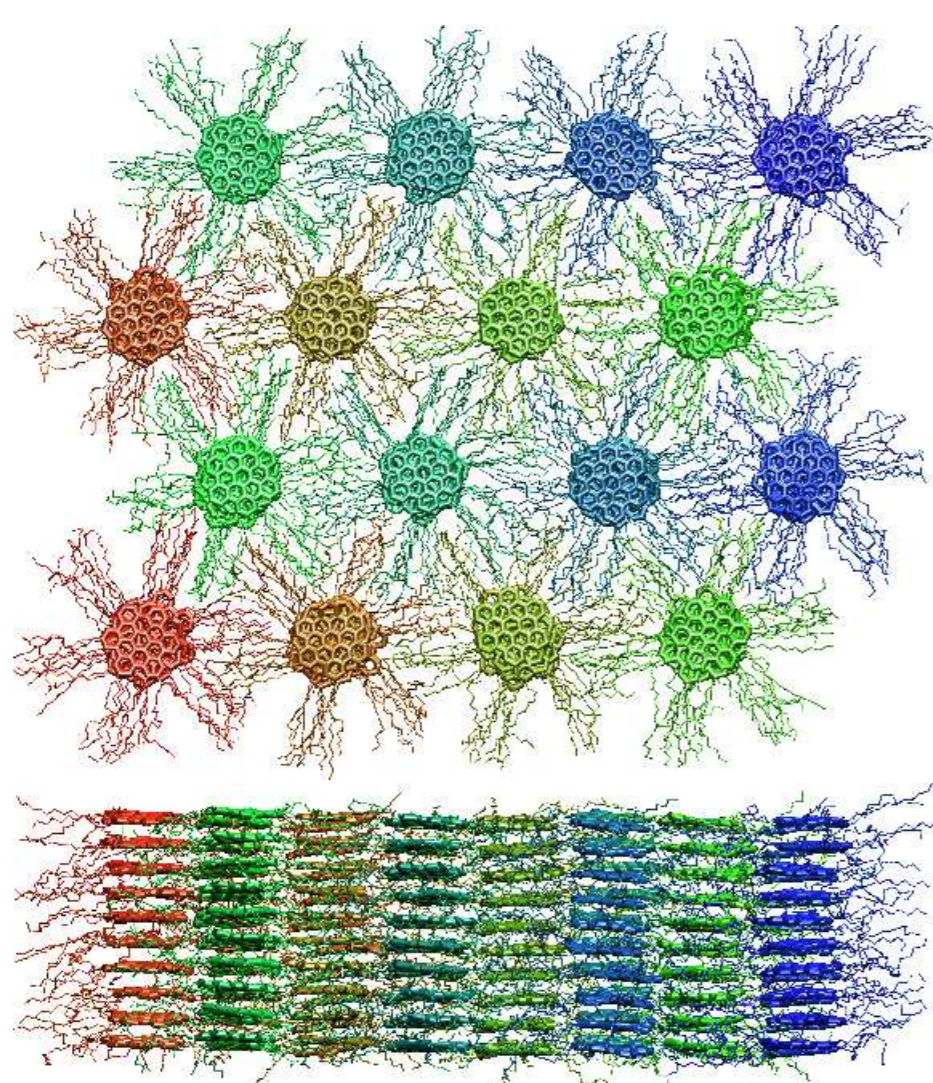
We study columnar phases of discotic liquid crystals (LCs) and their blends. The columnar phase consists of discs stacked on top of each other to form columns arranged in a two-dimensional (hexagonal or rectangular) lattice.



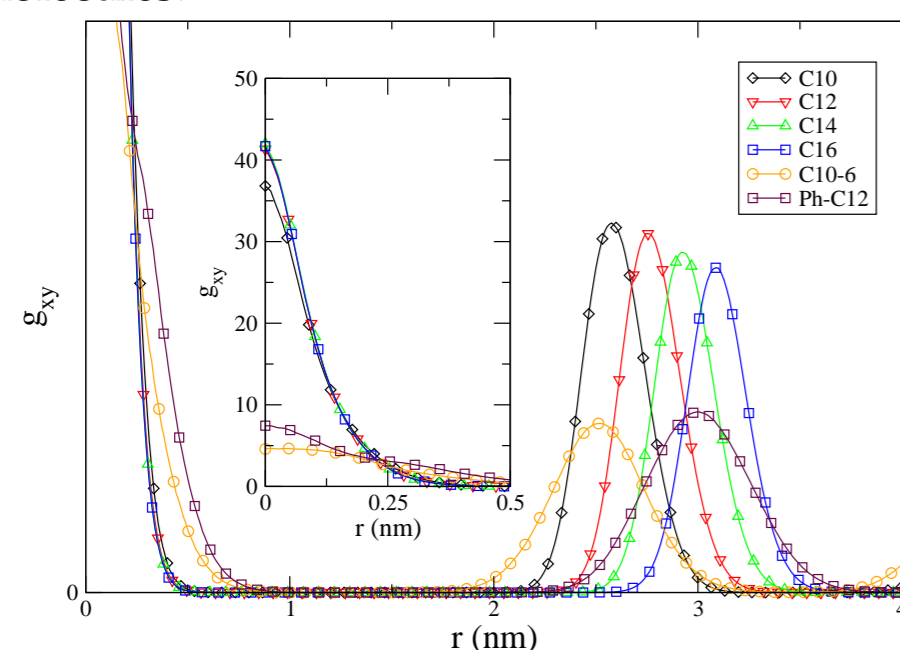
Hexabenzocoronene (HBC) and its derivatives (R = H, C10, C12, C14, C16, PhC12, C10-6).

MD simulations use OPLS force field [3]. Systems of 160 molecules arranged in columns of 10 molecules each are studied. We use Berendsen thermostat with pressure 0.1MPa and a temperature $T = 400K$.

$$E = \sum_{\text{angles}} \frac{1}{2} K_{\theta} (\theta - \theta_0)^2 \quad (1)$$
$$+ \sum_{\text{dihedrals}} \left[\frac{V_1}{2} (1 + \cos \phi) + \frac{V_2}{2} (1 - \cos 2\phi) + \frac{V_3}{2} (1 + \cos 3\phi) \right]$$
$$+ \sum_{\text{impropers}} K_d (\psi - \psi_0)^2$$
$$+ \sum_i \sum_{j>i} \left[\frac{q_i q_j}{r_{ij}} + 4\epsilon_{ij} \left\{ \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right\} \right]$$



Snapshots of a typical system (R = C12), poster, textop and side views. $T = 400K$. Perfect intra- and inter-columnar alignment of the molecules.

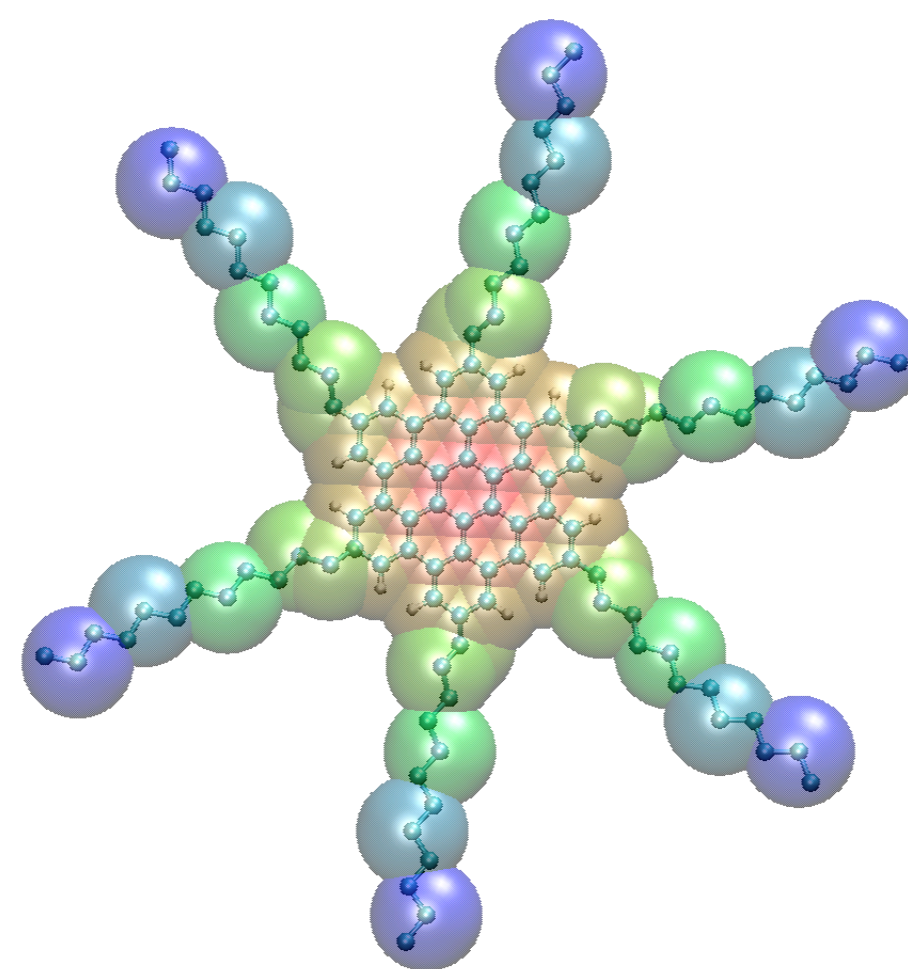


Positional correlation functions for all systems.

Current status: see Ref. [1]

Systematic coarse-graining

Different than atomistic MD simulation approach is required to study larger systems and to reach longer time-scales. Systematic coarse-graining is one of such approaches.



To reduce the number of degrees of freedom we first define the mapping points, and then derive the bonded and non-bonded interaction potentials for the point interaction centers. We assume that the probability distribution function of the system is a product of the corresponding probabilities

$$P(\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}) = \prod_{i=1}^N P(\mathbf{x}_i). \quad (2)$$

The coarse-grained potential for each variable can then be calculated as a Boltzmann inversion of the corresponding probability density distribution for this type of variable

$$P(\mathbf{x}_i) \sim \exp\left(-\frac{U(\mathbf{x}_i)}{k_B T}\right). \quad (3)$$

The probability density distributions are computed via Monte Carlo sampling of the atomistic structure of an isolated molecule. This sampling involves random moves of the coarse-grained variables, evaluation of the resulting total energy and acceptance based on a standard Metropolis criterion. The non-bonded potential of the coarse-grained system is again assumed to be a sum over all pairs, that is a non-bonded potential of a mean force can be approximated by simple pairwise potentials

$$U_{cg}^{nb} = \sum U_{ij}(\mathbf{r}_{ij}). \quad (4)$$

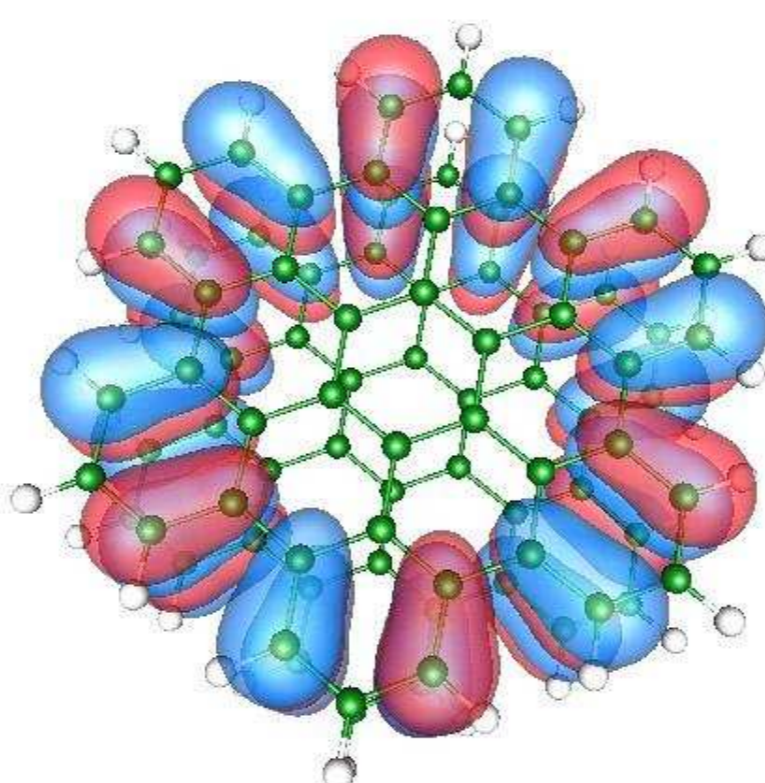
Current status: see Ref. [2] and Denis

Charge transport

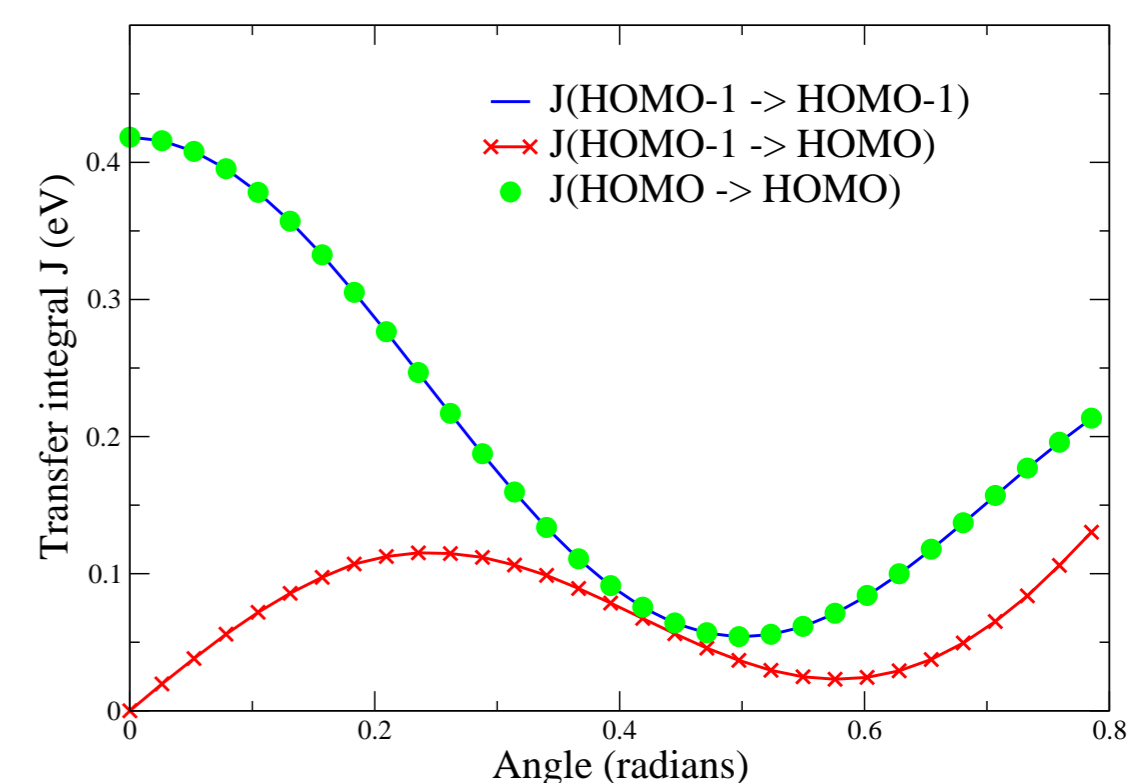
Charge transport is treated on a semi-classical level. Rates for the charge hopping are calculated using Marcus theorem [8]

$$W = \frac{4\pi^2}{h} \frac{J^2}{(4\pi\lambda k_B T)^{1/2}} e^{-\frac{(\Delta G - \lambda)^2}{4\lambda k_B T}} \quad (5)$$

where λ is the reorganization energy and J is the intermolecular transfer integral.



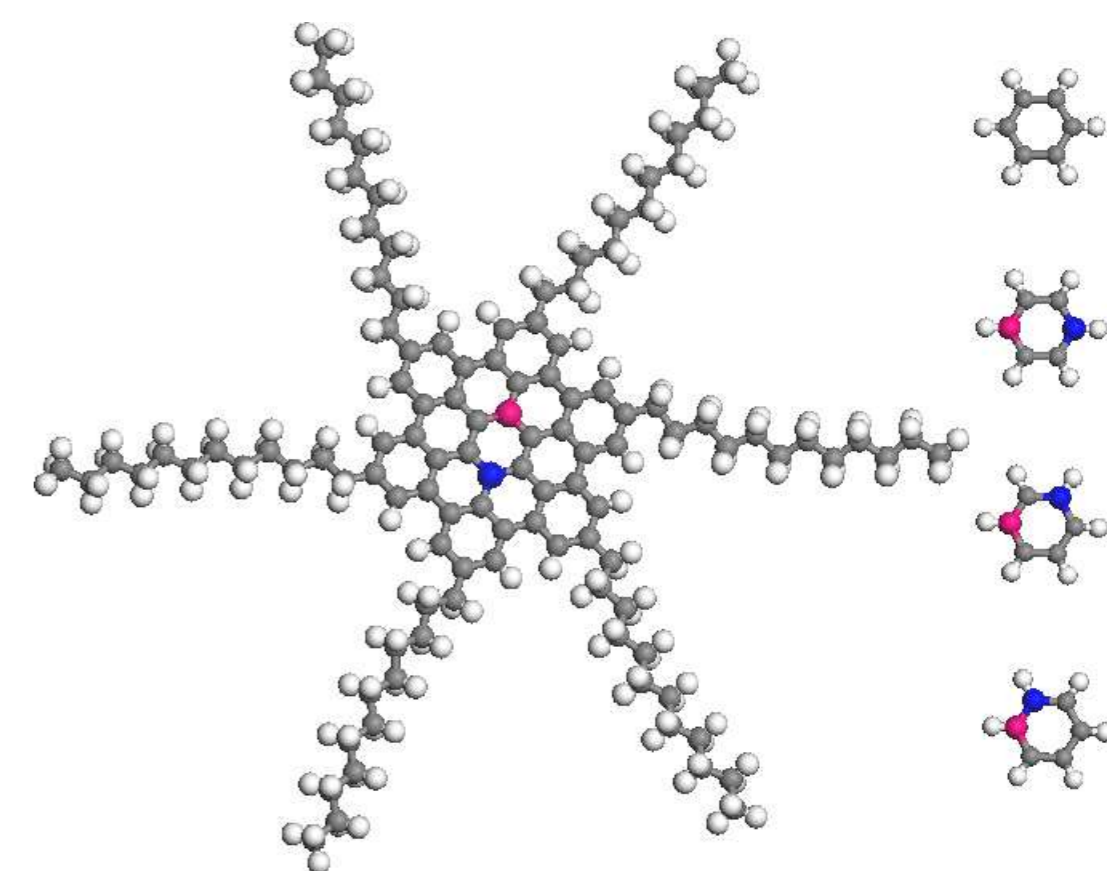
Calculation of the overlap integral from the HOMO, HOMO-1 energy levels difference. Geometry optimization: 6-31G* basis set; dimer wavefunction calculation: ZINDOS.



Transfer integrals J for a parallel pair of HBC molecules separated by 3.5 Angstroms. Because of the degeneracy of the top two orbitals, we show J for the HOMO to HOMO, HOMO to HOMO-1 and HOMO-1 to HOMO-1

Current status: see James

Rational compound design



We are working on the technique aiming at the design of the compounds with specific (optimized) physical properties. This, so-called rational compound design, allows to avoid screening of the high-dimensional chemical space spanned by all the possible combinations (stoichiometries) and configurations (isomers) of electrons and nuclei. At the moment we are testing the technique on small organic molecules (benzene) trying to understand how to dope hydrocarbons with a (B,N) pair so that the charge transport coefficients increase. Our final goal here will be to incorporate the multiscale method in the framework of the rational compound design and to predict and optimize the mobility of charge carriers in columnar phases of (B,N)-doped hexabenzocoronenes.

Current status: see Ref. [4] and a poster of Otto Anatole von Lilienfeld-Toal

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