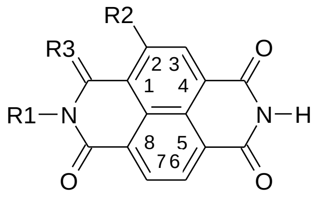
6×S for Chiral Semiconducting Naphthalene diimides:

Synthesis, Simulations, Structure, Spectroscopy, Spectroelectrochemistry, Sensors

Naphthalene diimide (NDI, Scheme 1) is an important core structure in the modern low molecular weight organic semiconductors. NDIs can exhibit both electron (n), hole (p) or ambipolar (n and p) types of conductivity, as well as electro- and photo-luminescence, photovoltaic and field effects. Thanks to their advantageous physicochemical properties large elastic surfaces can be covered with NDIs using different methods including simple printing techniques.

NDI



Scheme 1

Chirality brings molecules a new dimension. Enantiomers (two stereoisomers that are mirror images of each other) differ in *e.g.*: bioactivity; chiroptical spectra; interactions with chiral molecules; organoleptic properties. The chiral drugs gain an increasing economic rank. The global drug market is expected to reach ca. US$ 1 trillion in 2020, and enantiopure drugs will account for 95% of all chiral drugs. Pharmaceutical industry generates a need for advance in asymmetric synthesis, enantioselective separation and analysis, construction of chiral sensors, etc. Hence, chirality is very significant for modern chemistry, pharmacy, and medicinal chemistry and it is a great need for:

- development of sensitive monitoring of chiral molecules in different contexts;
- construction of a new class of chiral semiconductors;
- construction of new types of chiral sensors.

Chiral NDIs were studied infrequently and rather as amazing supramolecular structures. In the project we will attach chiral substituents in different positions of the NDI core. They are expected to selectively influence parts of the molecule connected with conducting electrons, holes, or both electrons and holes. The substituents will be additionally equipped with a proton-donor or a proton-acceptor group configured to effectively interact with a molecular target for sensing. NDIs exhibit good photo- and electro-luminescence properties and good invertibility of redox reactions. Hence, we can search for both: well-working optical and electrochemical enantioselective sensors.

The aim of the project is fivefold:

(**1**) To synthesize new chiral NDIs showing satisfactory n or p or ambipolar semiconductivity.

(**2**) To perform DFT simulations of conductivity-related properties, electron and chiroptical spectroscopy, and intermolecular interactions with chiral molecular targets for sensing.

(**3**) To make a comprehensive spectroscopy and X-ray diffractometry characteristic of the synthesized chiral compounds with an emphasis on use of chiroptical ECD, VCD and ROA techniques.

(**4**) To implement ECD, UV-vis, and EPR spectroelectrochemical measurements based on preceding voltammetric studies on type and invertibility of the reactions behind the chiral NDI conductivity.

(**5**) To construct optical and/or electrochemical enantioselective sensors for selected chiral targets.

To this aim we will: (a) develop new methods for synthesis of chiral compounds, (b) use new chiroptical spectroscopy methods which have never been used to study chiral semiconductors, (c) apply X-ray diffractometry which will help us to detect expected new supramolecular architecture of new compounds, (d) utilize electrochemistry methods typical for studies of organic semiconductors, (e) exploit spectroelectrochemistry methods including chiroptical circular dichroism which has never been used to study chiral semiconductors, and (f) construct new sensors, electrochemical or/and optical, selective toward important biological targets.

The study will be performed by very experienced scientists from the Institute of Nuclear Chemistry and Technology and from the Jagiellonian, Siedlce, and Warsaw Universities as well as Silesian Technical University in Gliwice.