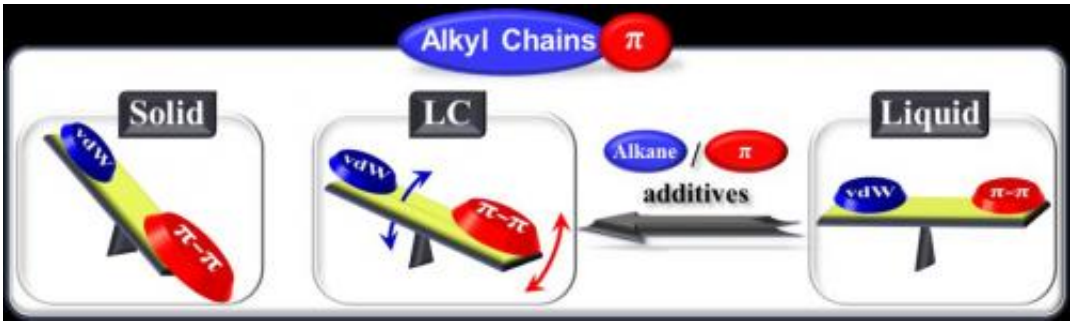
Optimising soft-optoelectronics materials through molecular engineering

March 24 2015



Credit: Sci. Technol. Adv. Mater. Vol. 16 (2015) 014805, Scheme 1.

The molecules used to make optoelectronic devices can be engineered to balance the chemical interactions within them and optimise their properties for specific applications, according to a review paper published in the journal *Science and Technology of Advanced Materials*. This paper, by researchers at the National Institute for Materials Science (NIMS) in Japan, proposes engineering strategies that could advance the manufacture of a range of devices.

Optoelectronic devices convert electricity into light, or light into electricity, and are integral to an increasing number of devices. For example, many television and mobile device displays are made with optoelectronic organic light-emitting diodes (OLEDs). Optoelectronics are also central to solar-powered devices, fibre optic communication and some electronic chips.

Many materials that are used to make optoelectronics consist of "π-conjugated" molecules that feature a complex form of chemical bonding in which many electrons are shared between many atoms. This bonding confers electronic and optical properties that are ideal for optoelectronics, but also leads to limitations. For example, at room temperature, most of these materials are solid and, therefore, unsuitable for flexible devices. What's more, π-conjugated molecules tend to be insoluble in solvents and difficult to work with in printing technology.

However, these properties can be changed by attaching alkyl chains to the π-conjugated molecules (alkyl chains have a backbone of carbon atoms, but can vary in length and branching structure). Scientists lack a complete understanding of how alkyl chains affect the properties of π-conjugated molecules, but Fengniu Lu and Takashi Nakanishi of NIMS have reviewed a range of studies to determine the fundamental rules of the process. (Since 2005, Dr. Nakanishi has himself invented a way to control the self assembly of linear alkyl chains, such as alkylated-fullerenes, to π-conjugated molecules. In addition, he recently developed an intriguing technique to create luminescent, room temperature "liquid" π-conjugated molecules by wrapping the π-moiety up with several branched alkyl chains.)

To assess the effects of attached alkyl chains, the NIMS team collated research that studied the properties of π-conjugated molecules modified with specific alkyl chains. Some studies demonstrated that different types of alkyl chains, solvent polarity, temperature and chain–substrate interactions led to the assembly of π-conjugated molecules into various two- and three-dimensional structures. Other studies showed that alkyl chains with certain structures allowed the formation of "thermotropic" liquid crystalline materials—which have properties between those of hard solids and soft liquids—as well as the formation of materials that were "isotropic" liquids at room temperature and from which photoconducting liquid crystals or gels could be formed. The authors

describe this strategy as "alkyl-π engineering" in their review article.

The researchers conclude that changes in the properties of alkylated-π molecules depend upon the precise balance of the interactions among the π-conjugated units as well as static interactions (known as van der Waals forces) among the alkyl chains. Different alkyl chains affect the balance of these interactions, leading to different molecular structures and properties. This insight will allow researchers to deliberately engineer π-conjugated molecules to have specific properties, making the production of high-performance optoelectronic devices more efficient.

More information: "Alkyl-π engineering in state control toward versatile optoelectronic soft materials." *Sci. Technol. Adv. Mater*. Vol. 16 (2015) 014805 DOI: 10.1088/1468-6996/16/1/ 014805

Provided by National Institute for Materials Science