

若干新型有机光电功能材料的分子设计、合成与性能 研究

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摘要

介绍本研究组得到国家自然科学基金资助的四个方面工作的进展。研究了金属有机化合物的结构与非线性光学性质的关系,总结了从分子几何构型着手,根据不同用途,对金属有机非线性光学材料进行分子设计的经验规律;提出了利用“组合式共轭桥”进行有机非线性光学发色团分子设计的新思路,所合成的几个有机化合物既有很大的光学非线性,又有紫移的最大吸收峰;通过化学键将有机发色团分子张到各种高分子的侧链上,

合成和表征了潜在的电光高分子和光折变高分子材料;采用无机-

有机夹层复合的思路对兼有导电性和强磁性的分子材料进行了探索,

将一些有机小分子和导电高分子分别插入了层状无机物MPS3的层间,得到了8个新的分子磁体,

而另一夹层化合物则表现了较高的电导率。

关键词 [有机材料](#) [夹心化合物](#) [非线性光学](#) [导电性](#) [光电材料](#) [磁性](#) [分子设计](#) [合成](#) [有机金属化合物](#)
[结构与性能关系](#)

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Molecular design, synthesis and properties of some new organic and organometallic electro-active materials

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Abstract Some basic research work on the synthesis, structure and properties of a variety of organic and organometallic electro-active materials was summarized. Synthesis, structure and nonlinear optical properties of organometallic compounds were studied systematically in this group. It was found that the molecular configuration formed by all the coordination atoms around the central metallic ions is one of the important factors that influence the linear and nonlinear optical properties of organometallic and coordination compounds. Based mainly on our own work, as well as some results from other research groups, an empirical rule which may help the design of new NLO materials from organometallic and coordination compounds for various applications was proposed. To design organic chromophores that exhibit both high nonlinearity and wide transparency, a new strategy of using "combined conjugation bridges" was proposed. Two organic chromophores designed by this new approach have shown a blue-shifted absorption and strong nonlinear optical property. Several electro-optical or photorefractive polymers were designed and synthesized. For this purpose, some functional moieties such as organic nonlinear optical chromophores and charge transporting agents were attached by covalent bonds to polysilanes, polysiloxanes, polyvinylcarbazoles, polyphosphazenes or polyferrocenylsilanes. Some polymers have demonstrated excellent performance and the others are waiting for the measurement results. A variety of organic ligands, electron-donating molecules and polyaniline were successfully inserted into the interlayer space of MPS3 (M=Mn or Fe) so as to explore the possibility of obtaining molecular conductive magnets. Eight intercalation compounds exhibited spontaneous magnetization with the Currie temperature of 30~60 K. On the other hand, the conductivity of some other intercalates was 5 to 8 orders of magnitude higher than that of the pure host.

Key words [SANDWICH COMPOUNDS](#) [NON LINEAR OPTICS](#) [ELECTRICAL CONDUCTIVITY](#) [PHOTOELECTRIC MATERIAL](#) [MAGNETISM](#) [MOLECULAR DESIGN](#) [SYNTHESIS](#) [ORGANOMETALLIC COMPOUNDS](#) [STRUCTURE AND PROPERTY CORRELATION](#)

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