FUNDING PROGRAM FOR NEXT GENERATION WORLD-LEADING RESEARCHERS

Project Title: Materials science of organic molecules with f-electron-like configuration	
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1. Background of research

Rare earth elements are of importance in many cutting-edge industrial materials.
This is due to critical roles of “f-electrons” in the elements in physical properties of the materials.
If the particular characters and behaviors of “f-electrons” could be realized even in the light elements without rare earth elements such as organic compounds, nothing to say, it greatly improves current science and technology.

2. Research objectives

Organic compounds have some advantages; possible control of molecular shape and tailor-made molecular array, etc. In our project, these are positively utilized to achieve “f-electron like configuration”, inspired by rare earth elements, using fully organic molecules.
The aim is to develop new organic materials with outstanding physical properties comparable to rare earth materials and to establish basic idea to design such kinds of materials without f-electrons.

3. Research characteristics (incl. originality and creativity)

Fortunately we have already found some organic electroactive materials with high localization of the spin and unexpected high magnetic property, similarly to materials bearing f-electrons.
Materials science of these organics has just started and thus we tentatively call them as “organic molecules with f-electron like configuration”.
These molecules show high potential to application in industry.

4. Anticipated effects and future applications of research

Light, abundant, low-toxicity, low-cost organic materials with outstanding physical properties would be very important to create new technology strongly contributing to development of next generation society. Future applications in energy-conversion and magnetic memory devices are especially expected to the materials.

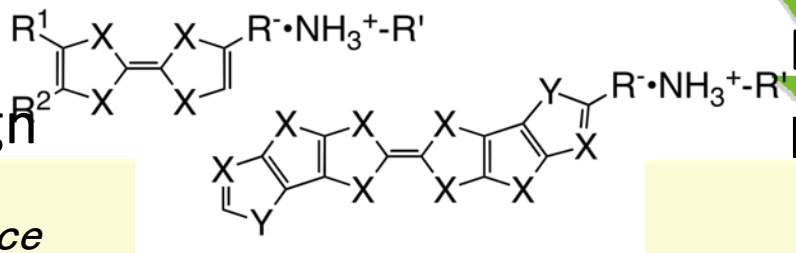
Research:

Novel organic electroactive materials have been developed, utilizing ammonium-doping technique. Characterization, physical properties, and electronic state of the materials are analyzed for future materials design.

Theoretical calculations

ab initio Molecular orbital calculations
First principles calculations

X = S, Se, Y = C, N
R = COO, SO_3, PSO etc.



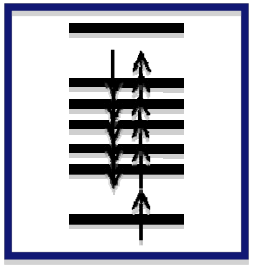
New materials design

Design for high performance
Powerful new donors
Application to soft materials
Synthesis of n-type conductors

Enhancement of physical properties

Electronic property
Magnetic property
Optical response
Thermoelectric property
Dielectric response

Unlimited target molecules



f-electron-like configuration

Characterizations

Doping level is analyzed by
NMR, IR, ESI-MS, ICP-MS,XPS and ESR
(NIMS, other facilities)

Structural analyses

Correlation between structure and properties
Single crystal structural analysis
Powder diffraction analysis
(KEK, SPring-8)