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Grant-in Aid for Scientific Research Areas
"Coordination Asymmetry"

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"Soft Crystal"

Magnetochemistry (MDPI)

JASCO

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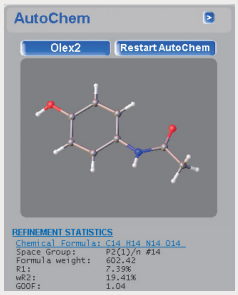
Break the size barrier!

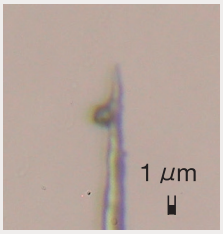
Think your crystal is too small for X-ray crystallographic analysis?

Think again! Even tiny microcrystals can yield full structures

A tiny (1 μm x 2 μm x 3 μm) crystal flake was selected from the powder contained in a pain killer capsule and subjected to single crystal structure analysis. After 30 min, AutoChem revealed the structure along with the absolute configuration, confirming that the crystal consists of acetaminophen.

Space group	$P2_1/n$
Chemical formula	$C_8H_9NO_2$
Formula weight / ASU	602.42
Total time Dose time	34 m 25 s 34 m 20 s
R_1 (%)	7.36
wR_2 (%)	19.09
Goodness of fit	1.04

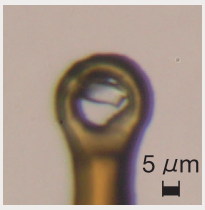




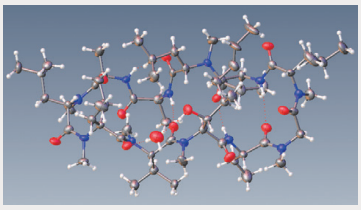
3 x 2 x 1 μm^3
Vol: 6 μm^3

Finish measurement before it decays

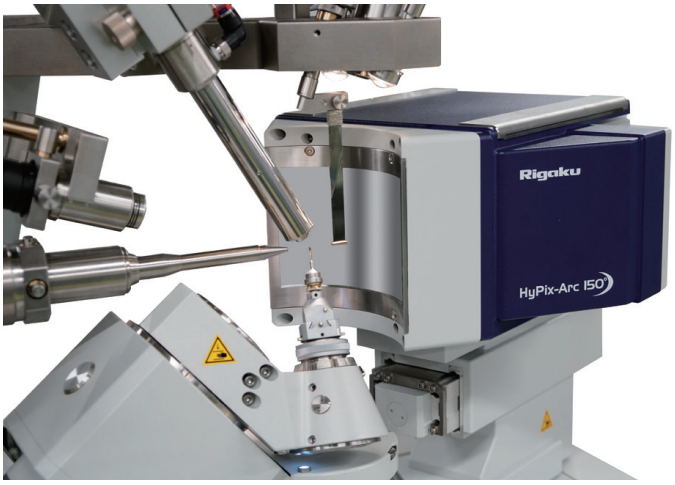
The structure analysis of cyclosporine A was a challenge because the crystal was small and rapidly damaged by X-rays. Nevertheless, accurate measurement of the weak anomalous signals was required because the drug consists of optically active amino acid derivatives. The HyPix-Arc 150° detector enabled structure determination in 2 hours because of its wide capture angle of diffracted X-rays.



25 x 10 x 6 μm^3
Vol: 1,500 μm^3



Cyclosporine A: $C_{62}H_{111}N_{11}O_{12}$
Molecular Weight: 1202.61
R_1=7.21%, Flack=-0.0 (2)



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- Dedicated analysis software BELMaster Ver. 7 enables the evaluation of not only BET and pore size distribution but also adsorption rates.

Applications: Cement, concrete, building materials, desiccant air-conditioning, low-temperature exhaust heat utilization, batteries

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	13.3Pa	3 units max	—	2 units
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Measurement range	N_2@77K	P/P_0=1E-8～0.997	P/P_0=1E-6～0.997	P/P_0=1E-8～0.997
	High pressure Adsorption	—	—	～950kPa
	H_2O	P/P_0=0.95@40℃	P/P_0=0.95@70℃	P/P_0=0.95@40℃

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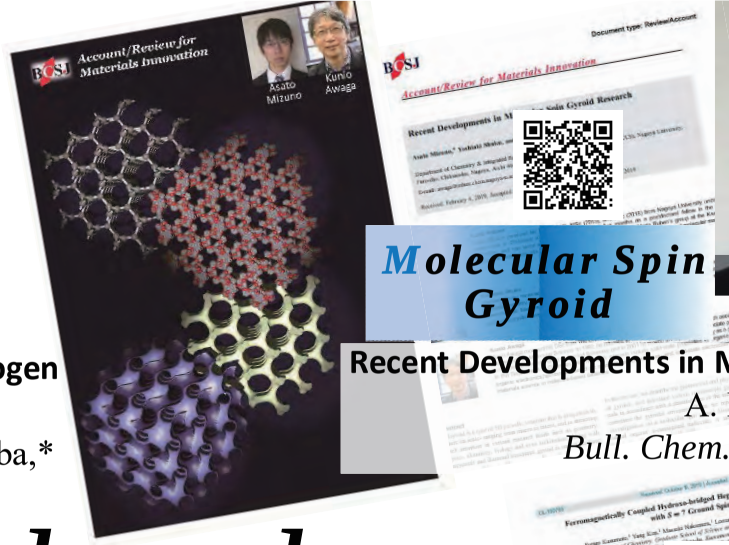
Molecular Magnetism

Nuclear Spin Conversion

【OPEN Access】

Swift and Efficient Nuclear Spin Conversion of Molecular Hydrogen Confined in Prussian Blue Analogs

Y. Ohtsubo, A. Mishima, A. Hori, R. Matsuda, R. Ohtani, M. Ohba,*
Chem. Lett. **2020**, *49*, 149-152.



Molecular Spin Gyroid

【OPEN Access】

Recent Developments in Molecular Spin Gyroid Research

A. Mizuno,* Y. Shuku, K. Awaga,*
Bull. Chem. Soc. Jpn. **2019**, *92*, 1068-1093.

Nanomagnets

Broadband-Millimeter-Wave Absorber Based on ε-$(Ti^{IV}Co^{II})_xFe^{III}_{2-2x}O_3$ for Advanced Driver Assistance Systems

A. Namai, K. Ogata, M. Yoshikiyo, S. Ohkoshi,*
Bull. Chem. Soc. Jpn. **2020**, *93*, 20-25.

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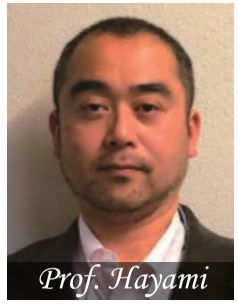
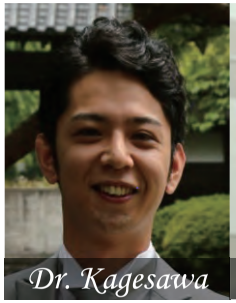
Ferromagnetic Interaction



Ferromagnetically Coupled Hydroxo-bridged Heptanuclear Ni(II) Wheel Cluster with *S* = 7 Ground Spin State

S. Kusumoto, Y. Kim, M. Nakamura, L. F. Lindoy,
S. Hayami,* *Chem. Lett.* **2020**, *49*, 24-27.



Spin-state Conversion

【OPEN Access】

Water-vapor Sensitive Spin-state Switching in an Iron(III) Complex with Nucleobase Pendants Making Flexible Hydrogen-bonded Networks

K. Kagesawa,* Y. Ichikawa, H. Iguchi, B. K. Breedlove, Z. Li,
M. Yamashita,* A. Okazawa, W. Kosaka , H. Miyasaka,*
Chem. Lett. **2019**, *48*, 1221-1224.

Organic π-Radical

【OPEN Access】

Trioxotriangulene: Air- and Thermally Stable Organic Carbon-Centered Neutral π-Radical without Steric Protection

Y. Morita,* T. Murata, A. Ueda, C. Yamada, Y. Kanzaki, D. Shiomi,
K. Sato, T. Takui, *Bull. Chem. Soc. Jpn.* **2018**, *91*, 922-931.

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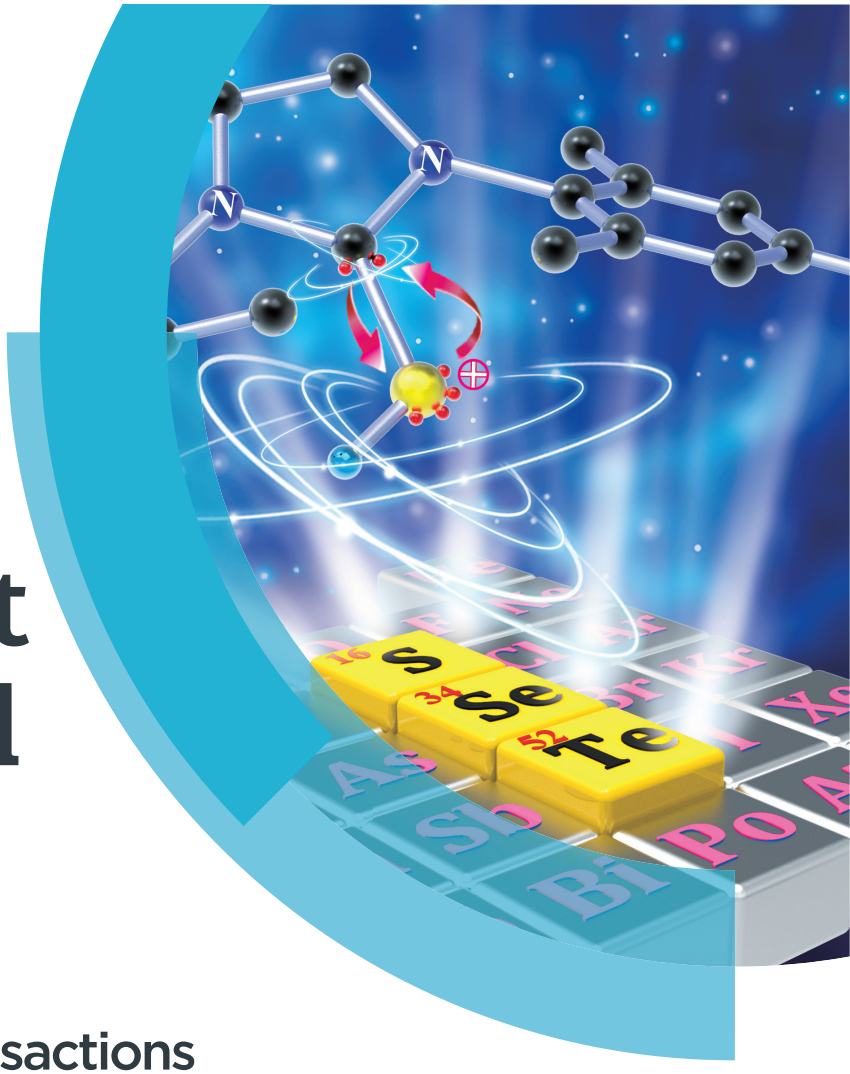

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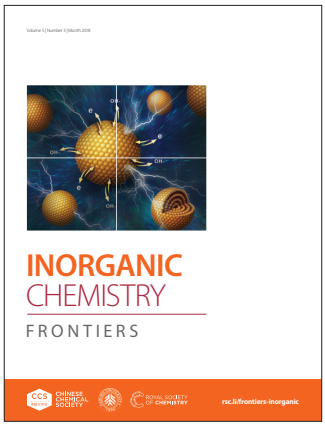

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"Scientific Research on Innovative Areas" for FY2016 - 20

Coordination Asymmetry:
Design of Asymmetric Coordination Sphere and Anisotropic Assembly for the Creation of Functional Molecules

"Coordination Asymmetry"

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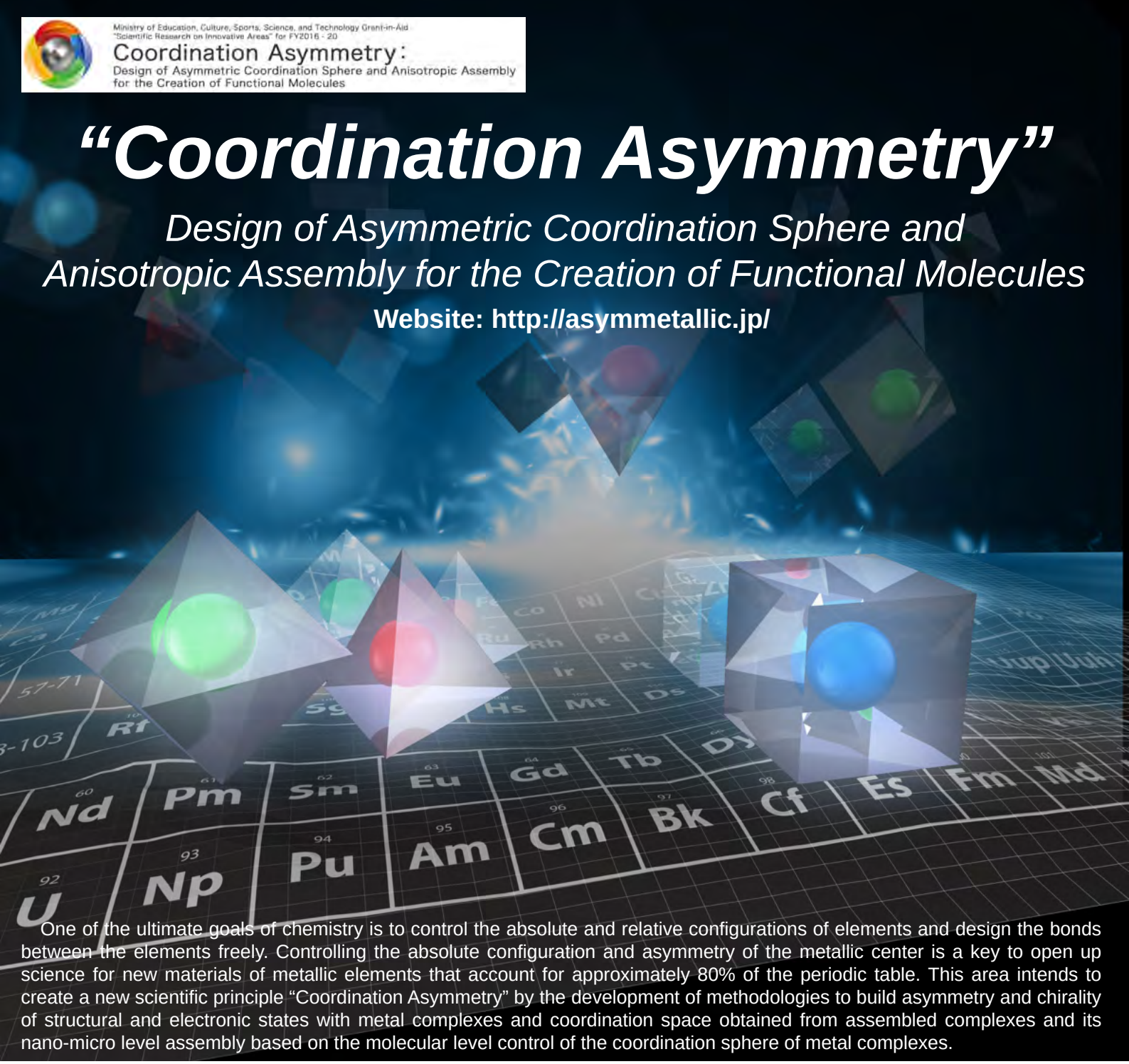
Website: http://asymmetallic.jp/



One of the ultimate goals of chemistry is to control the absolute and relative configurations of elements and design the bonds between the elements freely. Controlling the absolute configuration and asymmetry of the metallic center is a key to open up science for new materials of metallic elements that account for approximately 80% of the periodic table. This area intends to create a new scientific principle "Coordination Asymmetry" by the development of methodologies to build asymmetry and chirality of structural and electronic states with metal complexes and coordination space obtained from assembled complexes and its nano-micro level assembly based on the molecular level control of the coordination sphere of metal complexes.

A01: Molecular asymmetry

Leader: Mitsuhiko Shionoya (U-Tokyo)

Creation of higher-order molecular functions based on quantitative design of asymmetric coordination sphere

A02: Assembly asymmetry

Leader: Nobuo Kimizuka (Kyushu Univ.)

Creation of asymmetric high-order structures based on self-assembly and their functions

A03: Spatial asymmetry

Leader: Takashi Uemura (U-Tokyo)

Creation of asymmetric functional nanospaces exhibiting high selectivity, anisotropy, and directivity

A04: Electron system asymmetry

Leader: Toshiharu Teranishi (Kyoto Univ.)

Creation of chiral material conversion field and chiral electronic properties based on the asymmetrically assembled structures

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SOFT CRYSTALS

Grant-in-Aid for Scientific Research on "Innovative Areas" for FY 2017-21 (Area Number 2903)

Science and Photofunctions of Flexible Response Systems with High Order

Area Organizer
Professor Masako Kato (Department of Chemistry, Faculty of Science, Hokkaido University)

What is our project "Soft Crystals"?

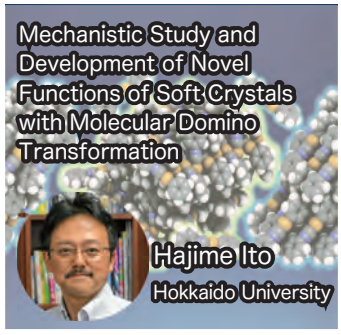
- Purpose of the Research Project -

This project aims to establish a new science concerning “Soft Crystals” , which responds to macroscopic gentle stimuli (e.g. vapor exposure, rubbing, and rotation) that exhibit visually remarkable changes such as luminescence and optical properties. This project also aims to develop novel functional materials on the basis of the scientific achievements. “Soft Crystals” are regulated solids with stable and highly ordered structures. However, they are characteristic of facile structural transformations and phase transitions in response to weak but particular stimuli . One of scientifically most important challenges is to clarify the phenomena of the formation and phase-transition of “Soft Crystals” . Through the scientific research, we aim to create a new area, which can provide new materials beyond the conventional hard crystals and/or soft matters.

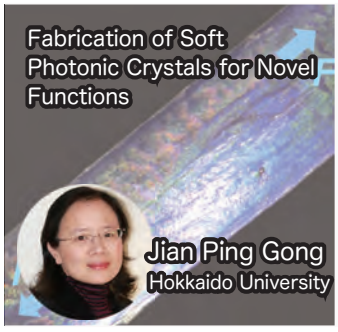
Contents of the Research Project

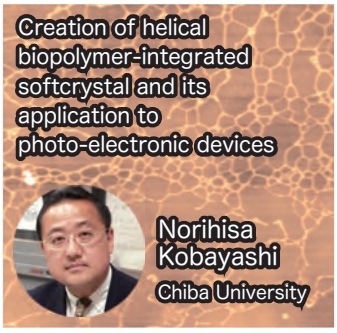
Research Item A01: Development of Soft Crystals through molecular design & synthesis

Research Item A02: Development of Soft Crystals with novel structure & morphology



Research Item A03: Development of Soft Crystals with superior physical properties & functions





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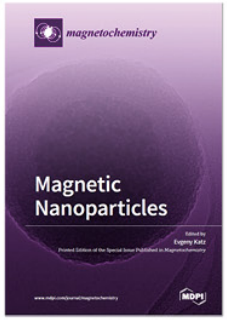

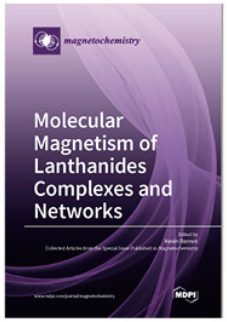

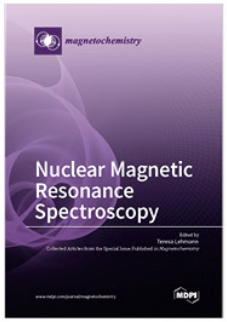

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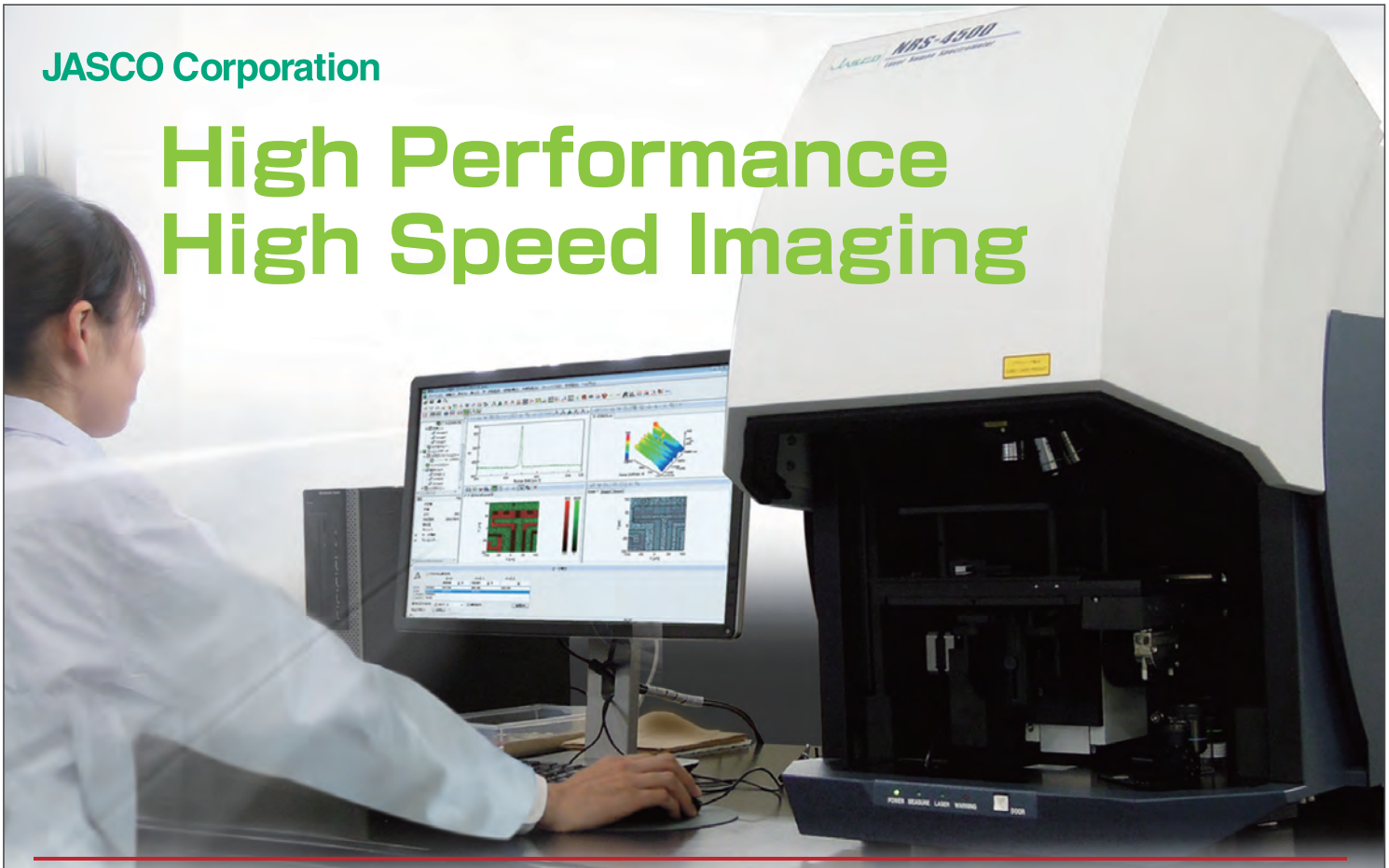

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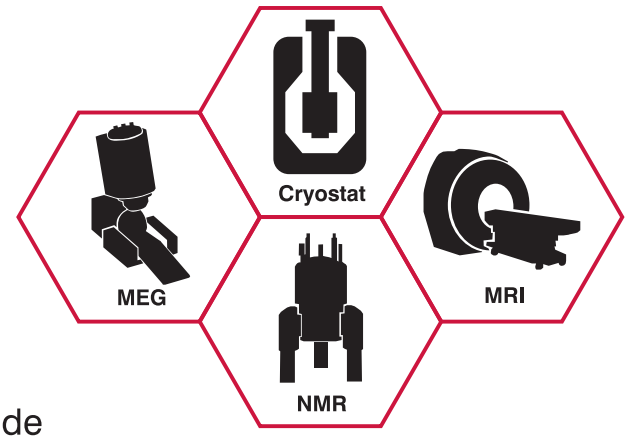

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