Exploration of Energy Conversion Materials by Ultrafast Screening Method

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Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

Brief overview

Materials for energy conversion including photoelectric functions are investigated by combination of advanced microwave spectroscopy (time-resolved microwave conductivity: TRMC) and materials informatics (MI). Our unique TRMC technique allows for a ultrafast screening of optoelectronic materials such as organic/inorganic films and even powder samples, the photoconductivities of which are correlated with device performances. On the basis of comprehensive understanding of fundamental properties of organic/inorganic materials and inductive correlation with output revealed by computer/data science, a breakthrough towards next-generation energy conversion materials is explored among the conventional and novel materials.

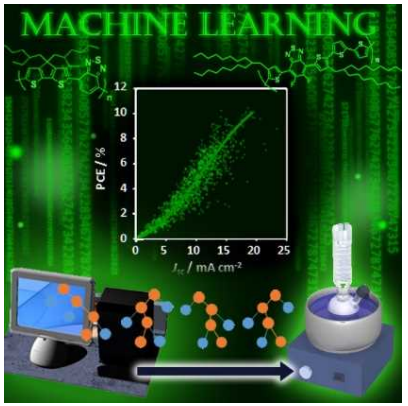

Fig. 1 MI-OPV

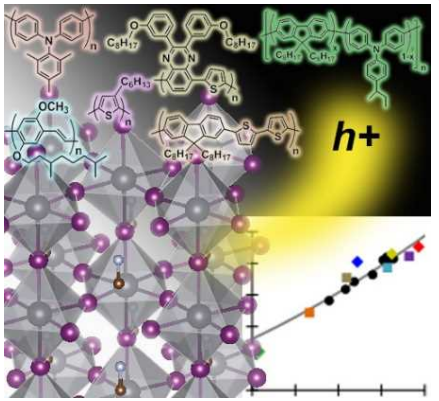

Fig. 2 PSC-Hole transfer

Achievement

By using MI and TRMC, we developed a new approach to organic photovoltaics (OPV) based on random forest machine learning (Fig. 1). Further, a direct evaluation of hole transfer yield from organic-inorganic lead-halide perovskite solar cell (PSC) to a hole transport layer (HTL) was performed, and the performance-governing factor was deduced from the statistical analysis of data science (Fig. 2). From an ultrafast experimental screening by TRMC, we found Bi_2S_3 powder shows an excellent photoresponse and developed its novel film-processing technique that provides improved film quality and optoelectronic properties (Fig. 3). We have also created a thermoresponsive material that exhibits emission switching upon heating and cooling (Fig. 4).

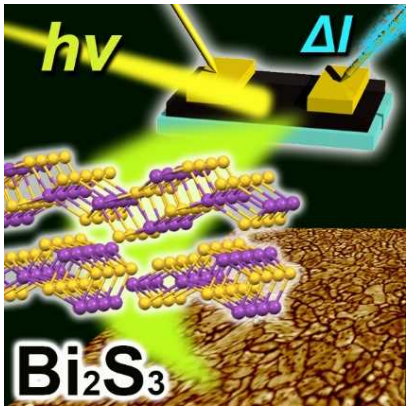

Fig. 3 Bi_2S_3 film

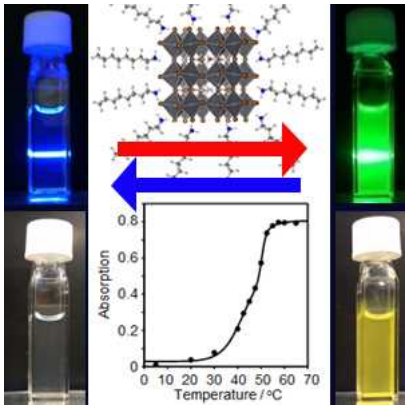

Fig. 4 Thermoresponsivity

Reference/Link

Group homepage http://www.chem.eng.osaka-u.ac.jp/~cmpc-lab/
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