Proton–electron-coupled Functionalities in Molecular Materials

Hatsumi Mori[1]

[1]*The Institute for Solid State Physics, The University of Tokyo, 277-8581 Chiba, Japan*
e-mail: hmori@issp.u-tokyo.ac.jp

Proton–electron-coupled reactions, specifically proton-coupled electron transfer (PCET), in biological and chemical processes have been extensively investigated for use in a wide variety of applications, including energy conversion and storage. However, the exploration of the functionalities of the conductivity, magnetism, and dielectrics by proton–electron coupling in molecular materials is challenging. Dynamic and static proton–electron-coupled functionalities are to be expected.

This presentation highlights the recent progress in the development of functionalities of dynamic proton–electron coupling in molecular materials [Fig. 1, 1-6]. Herein, single-unit conductivity by self-doping [1,2], quantum spin liquid state coupled with quantum fluctuation of protons [1,4,5], superconductivity related to proton quantum fluctuation, switching of conductivity and magnetism triggered by the disorder–order transition of deuterons [3], and their external responses under pressure and in the presence of an electric field are introduced [1]. In addition, as for the functionalities of proton–d/π-electron coupling in metal dithiolene complexes, magnetic switching with multiple PCET and vapochromism induced by electron transfer through hydrogen-bond (H-bond) formation is introduced experimentally and theoretically [1,6]. The basic and applied issues and potential challenges for development of proton-electron coupled molecular materials, functionalities, and devices are outlined.

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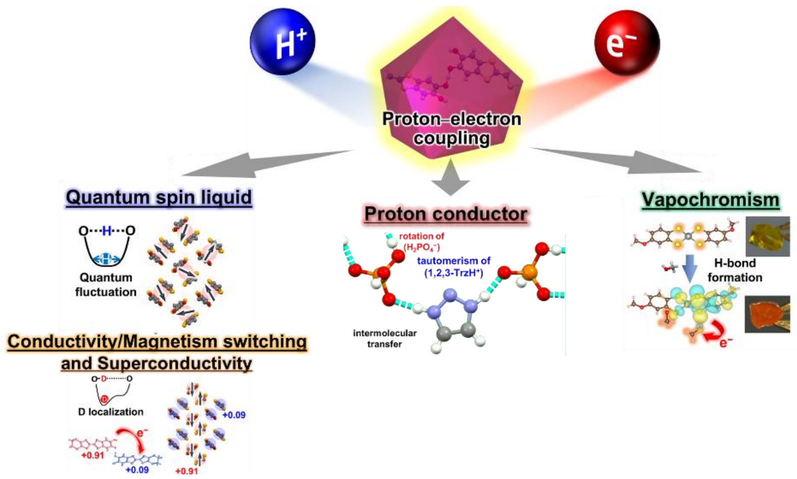

Fig. 1. Proton-electron coupled functionalities in molecular materials.

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