<u>Overcoming Liquid Hydrogen storage problem:</u> Increasing the *ortho-para* H₂ conversion yield

R. Muhida, Md. M. Rahman, M. David, W. A. Diño, H. Nakanishi, H. Kasai

Department of Precision Science & Technology and Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan

E-mail: rifki@dyn.ap.eng.osaka-u.ac.jp

One of the problems faced by engineers in using the hydrogen molecule for industry (e.g., aerospace, future vehicles) concerns the storage of liquid hydrogen, where special procedures are required to keep the composition (proportion) of the two types of hydrogen molecules known as orthohydrogen (o-H₂) and parahydrogen (p-H₂). Without these procedures, o-H₂ in the storage tanks slowly convert to p-H₂ over a period of days or weeks, releasing enough heat to evaporate most of the liquid. In order to limit the boil-off to low levels, it is necessary to fill the tank with liquid hydrogen that has already been converted to an equilibrium composition close to 100 % p-H₂. Thus, a method to increase the o-p H₂ conversion yield is important in liquid hydrogen storage [1-2]. In this study we introduce a new method to increase the o-p H₂ conversion yield on the catalysts surfaces by using:

[1]. Molecular orientation of H₂ on catalysts surface.

One of the ultimate goals of surface science is to be able to design and control reactions as they progress on surfaces. This entails an atomic-level understanding of the fundamental principles (elementary processes) underlying, among others, the bond-making and bond-breaking at surfaces. By using steric effect (SE) and dynamical quantum filtering (DQF) effect in the associative desorption and scattering of H₂ from surfaces we propose new reaction design of the *o-p* H₂ conversion on catalyst surfaces to increase the yield [3,4]. This design will give us higher catalytic surface area for the *o-p* H₂ conversion and improves the efficiency.

[2]. Design for new catalysts for o-p H₂ conversion by means of inhomogeneity of spin density distribution.

Based on our series of studies on magnetic properties of nanoclusters and its interactions with H₂ [5], we found that the inhomogeneity of spin density distribution can influence the *o-p* H₂ conversion yield [6]. This result gives us a promising possibility to increase this conversion by finding the best catalyst e.g., design of materials that can function as catalysts for the *o-p* H₂ conversion [7]. Inhomogeneity of spin density distribution thus can be considered as an important factor to look for the best catalyst for the *o-p* H₂ conversion.

References:

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