Orientational Effects in the Dissociative Adsorption Dynamics of H₂ on Li(100) Surface

N.B. Arboleda Jr.¹, H. Kasai¹*, W.A. Diño¹,² and H. Nakanishi¹

¹ Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan
² Physics Department, De La Salle University, Taft Ave., Manila 1004, Philippines

* Corresponding author’s e-mail address: kasai@dyn.ap.eng.osaka-u.ac.jp

Abstract

In recent years, Li-based complex hydrides (e.g. LiBH₄, LiNH₂) have attracted considerable attention because of their higher gravimetric hydrogen densities than those of conventional materials. Many studies on the Li-based complex hydrides aim to promote the hydrogen storage (desorption) reactions.¹⁻³ However, little is known about the interaction mechanism of hydrogen with Li and the behavior of hydrogen on and in the Li surface.

When H₂ approaches a metal surface, it may dissociate into 2 H atoms that are then absorbed into the surface. Thus, H₂ dissociation is one of the crucial steps in hydrogen absorption. As a first step in the study of the hydrogen storage process, we investigate the behavior of hydrogen on various surfaces by calculating the potential energy surfaces (PESs) for H₂ and the potential energy curves (PECs) for H on symmetric sites of the surface, with the aid of the density functional theory (DFT). We previously studied some hydrogen-metal systems⁴⁻⁷, and found that the energy barriers for H₂ dissociative adsorption are either small or negligible on the Ti, Ni, Pd and La surfaces (~0.1eV), while this is high on the Mg surface (~1.0eV). Also, the energy barriers for H absorption at three-fold hollow site are remarkably low for Mg and La (~0.4eV), comparatively low for Ti and Pd (~0.9eV), and high for Ni (~1.3eV). These can be attributed to the lattice structure of the substrates, where the distance between the lattice points is large, that is, the absorption hole area on the first layer is large, for the Mg, Ti, Pd and La surfaces (3.21Å, 2.95Å, 2.75Å and 3.76Å), as compared to the Ni surface (2.49Å).

We next focus on the hydrogen-Li system due to its suggested potentials as a hydrogen storage material. We have calculated the PESs for H₂ and the PECs for H at symmetric sites on a rigid Li(100) surface within the DFT⁸, and have introduced lattice relaxation on the substrate. We now perform a quantum dynamics study of the orientation effects in the dissociative adsorption of H₂ on the Li surface, the details of which we will discuss in the meeting.

References