

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**First-principles path-integral molecular dynamics study of diffusion process of hydrogen in face-centered cubic metals** HAJIME KIMIZUKA, SHIGENOBU OGATA, Department of Mechanical Science and Bioengineering, Osaka University — We investigated the H diffusivity in face-centered cubic Pd and Al by performing path-integral molecular dynamics (PIMD) modeling in the framework of density functional theory (DFT); in our calculations, we took nuclear quantum effects into consideration. The DFT results showed that the H-migration barriers ( $E_m$ ) in Pd and Al exhibited similar values (approximately 0.16 eV), while the H atoms were stable at octahedral (O) sites for Pd and at tetrahedral (T) sites for Al. The PIMD-based free-energy profiles for H migration between the O-site and T-site were evaluated using the thermodynamic integration of the centroid forces at 150-600 K. We confirmed that the quantum effects significantly affected the  $E_m$  and the difference between the energies of the H atom at the O-site and the T-site ( $E_{O-T}$ ); The  $E_m$  and  $E_{O-T}$  values in Pd at 300 K *increased* by 32% and 98%, respectively, relative to the classical limit. On the other hand, the  $E_m$  and  $E_{T-O}$  (i.e.,  $-E_{O-T}$ ) values in Al at 300 K *decreased* by 3% and 41%, respectively. This suggested that the quantum nature of H nuclei was essential for understanding the H-diffusion kinetics in these metals even above ambient temperature.

Hajime Kimizuka  
Department of Mechanical Science and Bioengineering, Osaka University

Date submitted: 05 Nov 2015

Electronic form version 1.4