Polarization dependence of palladium deposition geometry on ferroelectric $LiNbO_3$ (0001)

Seungchul Kim, and Andrew M. Rappe

The Makineni Theoretical Laboratories, Department of Chemistry,
University of Pennsylvania
Philadelphia, PA 19104-6323

Catalytic activity of transition metals supported by oxide depend on many details such as their size, shape, thickness, and supporting substrate. Although catalytic activity altering of Pd deposited on differently poled $LiNbO_3$ has been reported on 1984, its geometric structures and chemical properties are still open to debate. Using density functional theory (DFT) calculations, we investigate the geometric structure of palladium deposited on positively and negatively poled lithium niobate (0001). Geometries and energetics of Pd adsorption, diffusion, and clustering are presented. We discuss the possibility of different adsorption geometry on differently polarized surfaces, especially from the point of view of wetting and dewetting.

This work was supported by the US Department of Energy (DOE) through grant DE-FG02-07ER15920, and by the Air Force Office of Scientific Research (AFOSR) through FA9550-07-1-0397. Computational support was provided by the High-Performance Computing Modernization Office (HPCMO) of the US Department of Defense (DoD).