

Abstract Submitted
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Polarization dependent Pd deposition structure on LiNbO₃ {0001} surface¹ SEUNGCHUL KIM, ANDREW M. RAPPE, Department of Chemistry, University of Pennsylvania — We investigate effects of polarization orientation on atomic structure of palladium deposited on lithium niobate (LiNbO₃) {0001} surface, using density functional theory (DFT) and kinetic Monte Carlo (kMC) simulations. Adsorption, diffusion, aggregation and clustering process – include geometries, paths and energies – of Pd clusters were calculated from DFT simulations. It has been observed that energy barriers of Pd motions on the negatively poled (c^-) surface are much larger than those on the positively poled surface (c^+), which indicates the Pd motions on the c^- surface are much slower than that of c^+ surface. We demonstrate, using kMC with kinetic parameters from DFT, very slow motion of Pd on c^- surface leads dispersed small clusters or atoms while fast motion on c^+ surface leads large clusters, indicating larger Pd-covered area on c^- surface than c^+ after Pd deposition.

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