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Density-Functional Theory Study of Nucleation and Growth of Metallic Nanoparticles on MoS2(001) WISSAM A. SAIDI, Mechanical Engineering and Materials Science, Univ of Pittsburgh — The dispersion of metallic Pt nanoparticles (NPs) on MoS_2 monolayers is systematically analysed using first-principles density functional theory calculations. The nucleation of the NPs is followed step-by-step where we find that $n = 5$ is the cluster size where the growth of the NPs transforms from 2-dimensional (2D) to 3D. Owing to the topography of $MoS_2(001)$, the 2D NPs mostly attach to the support via a direct bonding with Mo atoms that sit in the troughs of the surface, while the 3D NPs are bonded to the sulfur atoms that are more extended in the vacuum region. Furthermore, we find that Pt is sufficiently mobile on the surface where the number of hopping events per second is $\approx 10^3$ s^{-1} along $[10\bar{1}]$ and ≈ 10 s^{-1} along $[1\bar{1}0]$ at room temperature. The somewhat large mobility suggests that monomer diffusion is not likely to be the rate-limiting step for Oswald ripening, and that Pt sputtering on $MoS_2(001)$ will result in large particles rather than a fine dispersion. The existence of a fast diffusion channel along $[10\bar{1}]$ suggests that the morphology of the NPs is anisotropic.

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