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Density functional theory study of methane dissociation over Pd nanoclusters

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Abstract content
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Palladium is often used as a catalyst for many processes in emissions control technologies [1, 2]. This is due to its potential of becoming a novel catalyst for low temperature methane combustion [3]. Palladium nanoclusters have a number of surface features and various adsorption sites, their relative activity play an important role if predictions are to be made for improved materials properties. The dissociation of methane over palladium nanoclusters and high index surfaces was investigated using density functional theory (DFT) as implemented in grid based projector augmented wave (GPAW) code [4]. Methane has been adsorbed on the Pd13 nanoclusters at various active sites, and the results shows that CH4 dissociate into CH3 and H. It is found that CH3 bind strongly to the top site forming a Pd-C bond of 2.06 Å and H on 3fold hollow with a Pd-H bond of 1.91 Å. Methane dissociation was found to be more favourable on the nanocluster than on Pd surfaces.

References

[1] C. Mateos-Pedrero, S.R. González-Carrazán, M.A. Soria and P. Ruíz, Catal. Today 203 (2013) 158-162
[2] M. Lyubovsky, S. Roychoudhury and R. LaPierre, Catal. Lett. 99 (2005) 113-117
[3] S.M. Lang, I. Fleicher, T.M. Bernhardt, R.N. Barnett and U. Landman, J. Phys. Chem. A 118 (2014) 8572-8582
[4] W. Kohn and L.J. Sham, Phys. Rev. A 140 (1965) 1133–1138

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