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Computational study of supported Pd catalyst for methane oxidation

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Abstract content
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Supported metal nanoparticles are at the heart of many industrial catalytic processes. Of particular significance are precious metal catalysts, which include the platinum group metals (PGM) for example Pt, Pd, Rh and noble metals such as Ag and Au. These metals find their way into processes as diverse as methane oxidation catalysts and emissions control technology [1-3]. A catalyst nanoparticle has a number of surface features, and it is important to know the relative activity of these different surface sites if predictions are made for improved materials. A pure metallic form of Pd was used to study the thermodynamics of the methane oxidation reaction over the flat Pd(111), Pd(100) and stepped Pd(211) surface. The calculations were carried out using the density functional theory (DFT) implemented within the GPAW code [4]. Reaction profile for methane oxidation on Pd(100), Pd(111) and Pd(211) shows similar trend indicating that both partial and complete oxidation are exothermic. It was also found that for all the possible reactions, the reaction profile of Pd(211) exhibit less adsorption energy and therefore the most preferred surface than Pd(100) and Pd(111) surfaces.

References

[3] C. Mateos-Pedrero, S.R. González-Carrazán, M.A. Soria and P. Ruíz, Catal. Today 203 (2013) 158-162

[2] C.R.K. Rao and D.C. Trivedi, Coord. Chem. Rev. 249 (2005) 613

[3] Y. Shao, J. Liu, Y. Wang and Y. Lin, J. Mater. Chem. 19 (2009) 46

[4] W. Kohn and L.J. Sham, Phys. Rev. A 140 (1965) 1133-1138

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