

On the thermodynamic stability of PdO-surfaces

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Although Palladium oxide is a compound of widespread technological interest with unique catalytic properties, only little is known about the structural and electronic properties of its surfaces. Not even the low-energy surface orientations are firmly established, that would then form the dominating facets of PdO particles. As a first step towards an understanding of the PdO surface structure, we therefore performed full-potential density-functional theory (DFT) studies of all (1×1) terminations of the low-index surfaces of tetragonal PdO using the program WIEN2k¹. Combining our DFT results with thermodynamics we discuss the composition, structure and stability of PdO orientations in equilibrium with an arbitrary oxygen environment. Special emphasis is put on a thorough comparison of the traditional linear augmented plane wave (lapw) method with the recently developed augmented plane wave plus local orbitals (apw+lo) scheme². For both bulk and surface studies we find that the apw+lo method allows to significantly decrease the employed basis set at the same level of convergence, thereby reducing the required CPU time by almost a factor of 2.

¹P. Blaha et al., WIEN2k, Techn. Universität Wien, Austria, 2001, ISBN 3-9501031-1-2

²E. Sjöstedt *et al.*, Solid State Commun. **114**, 15 (2000).