Bonding and Stability of the Phosphonate Group on the Polycrystalline Cerium Oxide: Effect of the Deposition Technique, Non-functional Group and Temperature

V. Kalinovych[1], L. Piliai[1], Y. Kosto [1], S. L. Mehl[2], T. Skála[1], I. Matolínová[1], K. C. Prince[2], N. Tsud[1]

[1] *Charles University, Faculty of Mathematics and Physics, Department of Surface and Plasma Science, V Holešovičkách 2, Prague, 18000, Czech Republic*

[2] *Elettra-Sincrotrone Trieste S.C.p.A., in Area Science Park, Strada Statale 14, km 163.5, Basovizza (Trieste), 34149, Italy*

Email address of corresponding author kalinovych.viacheslav@gmail.com

In this work, we studied the adsorption and stability of the phosphonate group (R-PO(OH)$_2$) on polycrystalline cerium oxide as a function of such parameters as deposition technique, non-functional group (R) and thermal treatment.

The effect of the non-functional group was investigated using two molecules with similar structure phenylphosphonic acid (PPA) (Fig. 1a), consisting of phenyl ring and phosphonate group, and hexylphosphonic acid (HPA) (Fig. 1a), consisting of 6 C atoms alkyl chain and phosphonate group. Two deposition methods were compared, molecular deposition in ultra-high vacuum using the Knudsen cell (for PPA only) and deposition from methanol solution. The changes in the stability and bonding of the phosphonate group were studied in the temperature range *25 °C - 450 °C*. All the systems were characterized by resonance photoelectron spectroscopy, X-ray photoelectron spectroscopy and near-edge X-ray adsorption fine structure spectroscopy.

The result of that experiment demonstrates that:

- PPA and HPA bind to the surface through the phosphonate group in tridentate geometry independently of deposition technique and non-functional group.
- The phosphonate group on CeO_2 is more stable for adlayers deposited from methanol solution (Fig. 1 b). PPA deposited in UHV desorbs/decomposes constantly upon annealing (Fig.1. b, c red line). While PPA deposited from solution demonstrates higher stability up to 400 ℃ (Fig.1. b, c blue line).
- The stability of the phosphonate group is affected by the non-functional group of a molecule. HPA with an alkyl chain (Fig. 1. green line) is less stable than PPA deposited from methanol solution and decomposes/desorbs after 225 ℃.

The Grant Agency of Charles University in Prague (project 314123) is acknowledged for financial support.

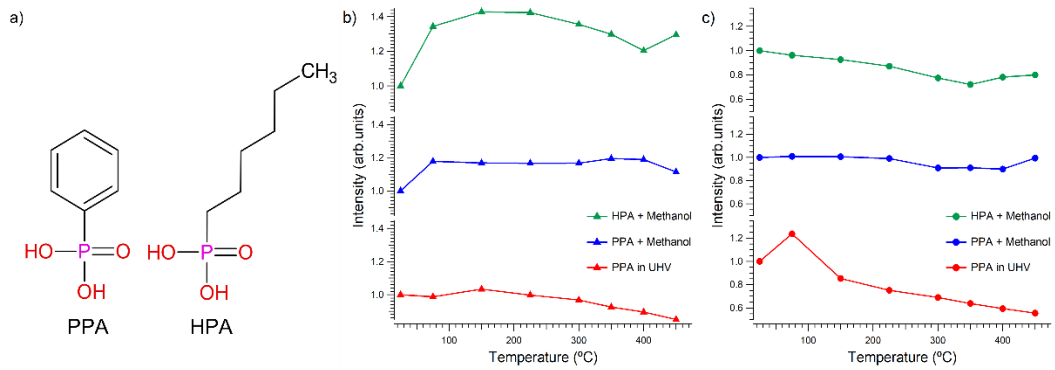

Fig. 1. a) Phenylphosphonic acid and hexylphosphonic acid; signal intensity evolution of b) P 2p and c) C 1s core levels measured using 230 eV and 410 eV photon energy, respectively.