

Slab Plane wave model for the adsorption of Pt on cubic and tetragonal ZrO₂ (001) Solano, J. G.^{1,2}, Gil Rebaza, A. V.³ and Taft, C. A.²

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We have used the plane wave pseudopotential method of Vasp to investigate the adsorption of Pt on cubic and tetragonal surfaces of ZrO₂ (001). Our calculations are performed in the framework of density functional theory using the Ultrasoft Pseudopotential and Projector Augmented Wave with the Perdew and Wang 91 (GGA) and PBE approximation to the exchange correlation functional. Starting from the bulk we use 8 layer models terminated in oxygen with a vacuum of 12.58 Å. The adsorption calculations were done for different sites of adsorption. For the cubic (001) surface we investigated the following sites: a) oxygen atom perpendicular to the surface b) hole (hollow) between 4 oxygen atoms in the center of the cell with a Zr atom below the second layer c) between two oxygen bridge atoms. For the tetragonal surface (001) we investigated the position of adsorption a) above the oxygen atom perpendicular to the surface b) above the oxygen atom of the second layer c) between the two oxygens of the first layer d) between the two oxygens of the second layer. We determined the adsorption energies for each site of the cubic and tetragonal surfaces. We also investigated the charge densities in the (010) and (100) directions of both surfaces for the Pt-surface right after adsorption in the (100) and (001) directions for each adsorption site. Our results indicate that the adsorption energies and the inter atomic distances Pt-surface depends on the crystallographic phases of the surface cut and on the geometrical adsorption sites.

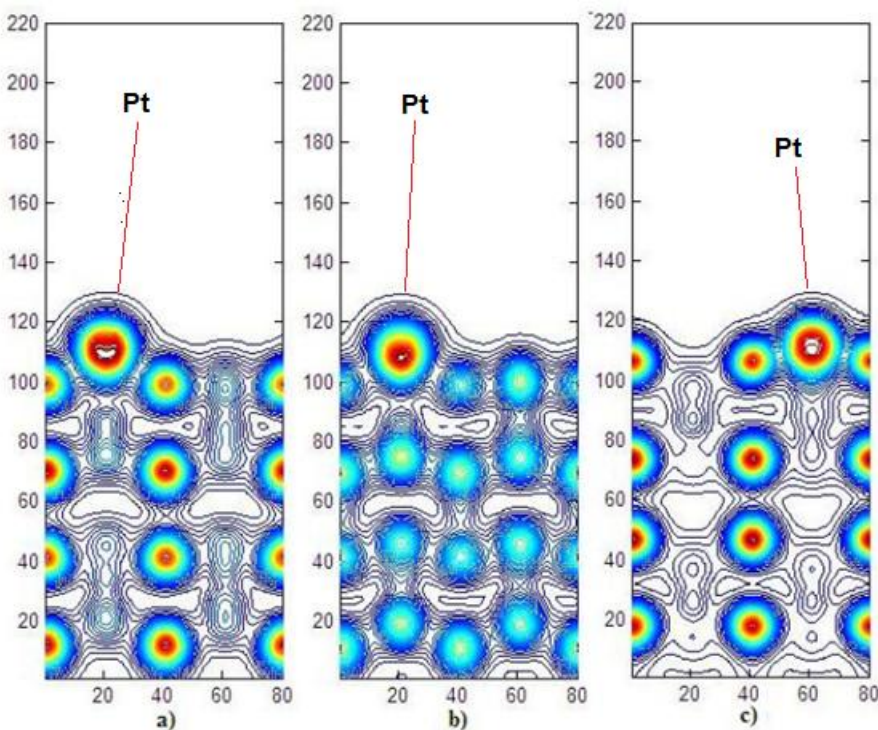


Fig. 1 Charge density of Pt adsorbed on c-ZrO₂ (hollow)

References

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