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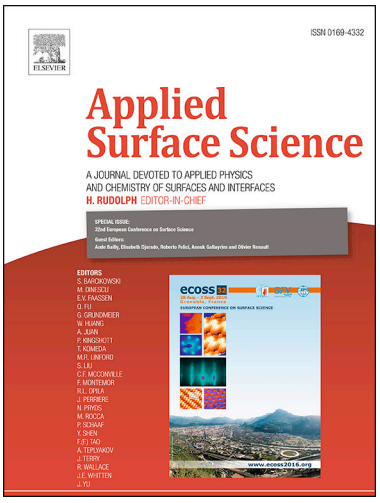

Full Length Article

The adsorption and dissociation of O_2 on Pd and Pt modified TaC (100) surface: A first principles study

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The adsorption and dissociation of O_2 on Pd and Pt modified TaC (100) surface: A first principles study

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ABSTRACT: The adsorption and dissociation of O_2 on the palladium and platinum modified TaC (100) surfaces were investigated based on the density functional theory calculations. It is found that the adsorption sites of O_2 are the Ta-Ta bridge sites on both the partially covered TaC (100) surfaces by Pd and Pt, M_4/TaC (100) (M = Pd and Pt), while the 4-fold metal hollow sites and the metal-metal bridge sites are preferred on the fully covered TaC (100) surfaces by Pd and Pt monolayer, M_{ML}/TaC (100), respectively. The deposition of Pd or Pt can enhance the oxidation resistance of TaC (100). Meanwhile, the TaC (100) decorated by monolayer Pd still exhibited outstanding catalytic activity for O_2 dissociation. Our study might be useful to designing efficient catalysts for the oxygen reduction reaction.

Keywords: noble metal decoration; TaC; oxygen dissociation; oxidation resistance; density functional theory

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