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\*\*\*\*\*All the revisions are shown in BLUE \*\*\*\*\*

**The adsorption and dissociation of O<sub>2</sub> on Pd and Pt modified TaC (100) surface: A first principles study**

Yanan Meng<sup>a</sup>, Xilin Zhang<sup>a</sup>, Jianjun Mao<sup>a</sup>, Xiaopei Xu<sup>a</sup>, and Zongxian Yang<sup>a\*,b</sup>

<sup>a</sup>College of Physics and Materials Science, Henan Normal University, Xinxiang, Henan

453007, China

<sup>b</sup> National Demonstration Center for Experimental Physics Education (Henan Normal

University), Xinxiang, Henan 453007, China

**ABSTRACT:** The adsorption and dissociation of O<sub>2</sub> 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<sub>2</sub> are the Ta-Ta bridge sites on both the partially covered TaC (100) surfaces by Pd and Pt, M<sub>4</sub>/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<sub>ML</sub>/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<sub>2</sub> 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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\* Correspondence author. E-mail: [yzx@henannu.edu.cn](mailto:yzx@henannu.edu.cn) (Z Yang)

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