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Oxidation of Pt (100) surface: Ab initio studies[1] EUNJA KIM, DAVID STUCKE, TAO PANG, Department of Physics, University of Nevada, Las Vegas, NV 89154 — We have performed density-functional calculations to investigate the oxidation process of Pt (100) surface. We carefully examine the previously proposed models and propose a new dissociative model of oxygen molecules on the Pt (100) in this study. Our findings also indicate that one monolayer of oxygen atoms can be covered on Pt (100) surface with 1.09 eV/O_2. The role played by oxygen and temperature in the degradation of catalyst will be further discussed in details.

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