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First-principles study of the oxygen-reduction reaction on the Pt (100) surface[1] EUNJA KIM, TAO PANG, Department of Physics and Astronomy, University of Nevada, Las Vegas — We have performed density-functional study of oxygen-reduction reaction on the Pt(100) surface. Equilibrium structures of oxygen on the surface are found and carefully analyzed. Our calculations show that oxygen molecules reduce into atoms when they reach the Pt(100) surface and cover the surface up to a complete monolayer with a binding energy of 2.12 eV per oxygen atom. More oxygen molecules reaching the surface will continue to reduce but also drive the ones in the monolayer away from the surface, making the surface an effective catalyst. However, oxygen does not stack up into layers on the Pt(100) surface and therefore does not play a significant role in degrading the Pt (100) surface during any catalytic process there.

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