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Density-functional study of Cu atoms, monolayers, films, and coadsorbates on polar ZnO surfaces

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The structure and electronic properties of single Cu atoms, copper monolayers, and thin copper films on the polar oxygen and zinc terminated surfaces of ZnO are studied using periodic density-functional calculations. We find that the binding energy of Cu atoms sensitively depends on how charge neutrality of the polar surfaces is achieved. Bonding is very strong if the surfaces are stabilized by an electronic mechanism which leads to partially filled surface bands. As soon as the surface bands are filled (either by partial Cu coverage, by coadsorbates, or by the formation of defects), the binding energy decreases significantly. In this case, values very similar to those found for nonpolar surfaces and for copper on finite ZnO clusters are obtained. Possible implications of these observations concerning the growth mode of copper on polar ZnO surfaces and their importance in catalysis are discussed.

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