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Origin and application of the "lattice distortion energy" spent upon chemisorption[1] MARISOL ALCANTARA ORTIGOZA, SERGEY STOLBOV, University of Central Florida — We reveal the origin of the "inertness" of gold toward atomic and molecular oxidizing agents. Contrasting with the fact that Au forms very stable alloys and can certainly be activated under certain circumstances, such nobleness has long been attached to the weakness of the adsobate-metal interaction. Not surprisingly, e.g., from all transition-metal surfaces, Au stands for the weak binding energy of atomic O. We have shown that the origin of gold's unique corrosion resistance is the combination of several factors but, contrary to what one would expect from its "nobleness," is mainly caused by the unusually large perturbation on Au-Au bonds upon O adsorption that reduces the binding energy by what we call the "lattice distortion energy." In this work, we shall show that the "lattice distortion energy" is particularly high for Au because of the relatively deep position and broad width of its d-band. The latter unique feature allow for a strong interaction between Au d-states and oxygen p-states, which in turn strongly weaken Au-Au bonds. The "lattice distortion energy" is always present but has been neglected altogether in understanding or designing catalysts. We thus propose to utilize this new degree of freedom for this purpose.

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