

Supplementary Information

Why are Zn-rich Zn-Mg nanoalloys optimal protective coatings against corrosion? A first-principles study of the initial stages of the oxidation process

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1 Nucleophilic Fukui function f^-

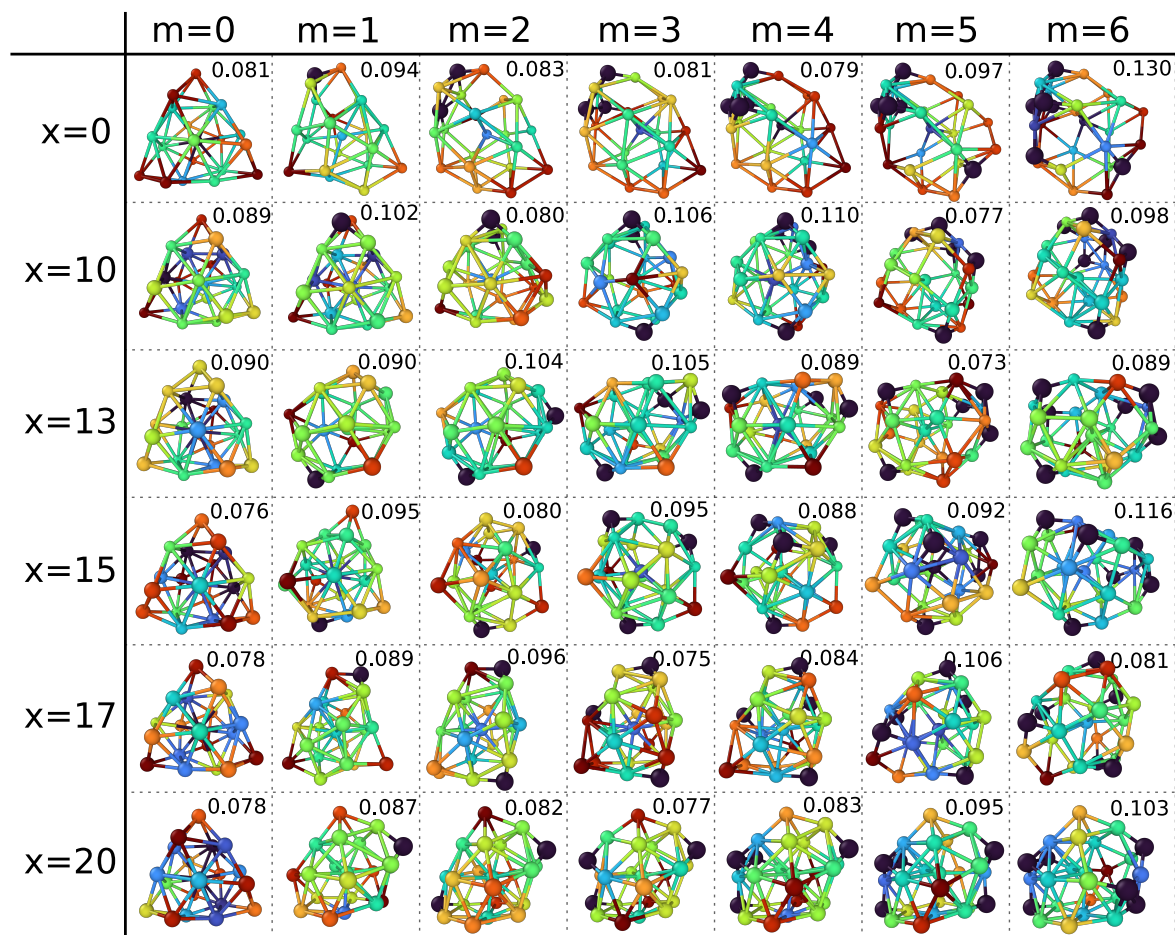


Fig. S1. Condensed Fukui functions f^- for $\text{Zn}_x\text{Mg}_{20-x}\text{O}_m$ nanoalloys. Oxygen atoms show the smallest value possible (dark blue balls), while the largest f^- value is shown for every structure. Small and large colored balls are Mg and Zn atoms, respectively.

The nucleophilic Fukui function f^- is depicted in Figure S1 for the set of 42 $\text{Zn}_x\text{Mg}_{20-x}\text{O}_m$ clusters. The O atoms, that are not supposed to be prone to electrophilic attack, are assigned a f^- value equal to 0 for ease of visualization (this way, all of them have the same dark blue color in the figure). Their true f^- values are always significantly lower than those of magnesium or zinc surface atoms, but of the same order of magnitude as for the central atom

of the cluster which is protected by the surface layer and, as such, is weakly reactive.

2 Oxygen adsorption energy

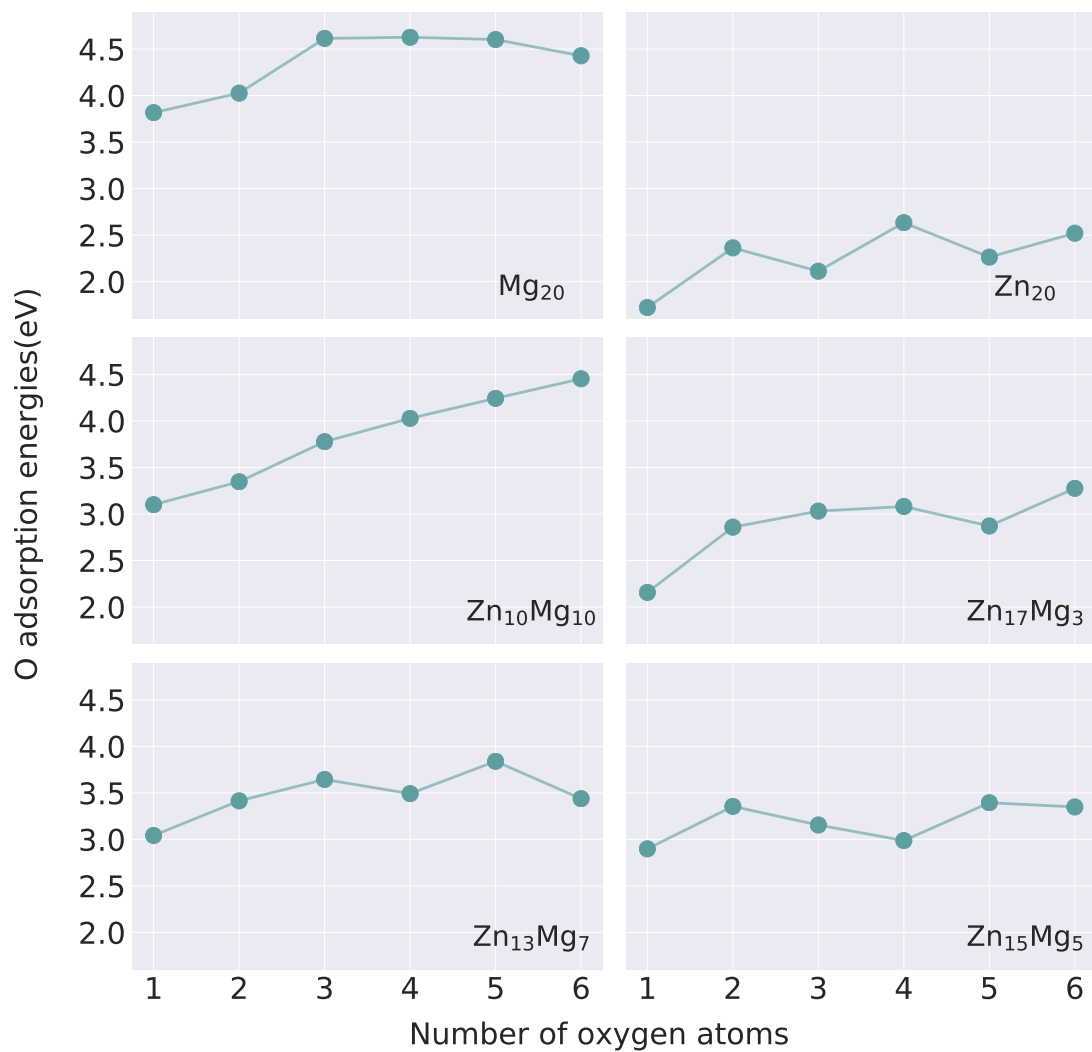


Fig. S2. Adsorption energy of the newcomer oxygen atom as a function of the oxygen content, for all the compositions under study.