Theoretical study of the interaction of molecular oxygen with copper clusters

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A new method based on frontier orbital theory has been used to investigate the binding site of molecular oxygen to neutral and anion copper clusters. It has been shown that one can make useful predictions of the binding sites based on the knowledge of the donor local reactivity of the cluster using the condensed Fukui function, fFf. In this way, it was found that Cu 3, Cu5, and Cu5- have the highest reactivity toward molecular oxygen.