Density functional theory characterization of the formation of copper clusters on Fs and Fs+ centers on a MgO surface

Florez, Elizabeth

Mondragón, Fanor

Truong, Thanh N.

Fuentealba, Patricio

Electronic structure and chemical reactivity of Cun clusters (n = 1-4) supported on a regular site (O5c) and on an oxygen vacancy (Fs and Fs+) of the MgO (1 0 0) surface were investigated using density functional theory. It was found that neutral oxygen vacancies, Fs centers, are good trapping sites for Cu atoms and nucleation centers while Fs+ centers are not. Both, first ionization potential and the chemical reactivity present odd-even oscillations in the free and supported clusters, these oscillations are related to the electronic nature of the layer open/closed for clusters with odd and even n, respectively, this behavior is similar for supported clusters on an Fs center compared with free clusters. It is also found that the ionization potential and the chemical reactivity are modified when the clusters are supported on the MgO vacancies.