

Electronic Supplementary Information for the article Cu adatom charging on Mo supported ScN, MgO and NaF

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1 Supplementary information to the subsection *Distortion induced charge localisation on AB/Mo surface*

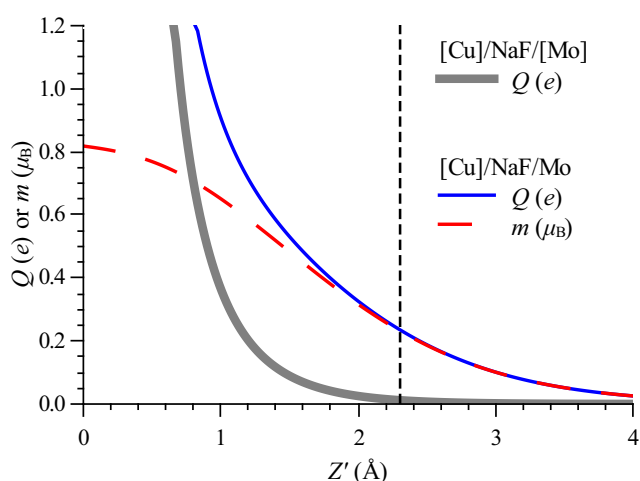


Figure S1: The comparison of [Cu]/NaF/[Mo] with [Cu]/NaF/Mo showing charge spillover for the latter. Charge and magnetisation were integrated between the $z = Z'$ plane and the middle of the vacuum gap. $Z' = 0$ corresponds to the z coordinate of [Cu]/NaF/Mo surface termination.

The spatial distribution of charge accumulated in [Cu]/NaF/Mo was examined further. In Fig. S1 we show charge density for [Cu]/NaF/Mo and [Cu]/NaF/[Mo] integrated along the Z axis. Let us recall that both [Cu]/NaF/Mo and [Cu]/NaF/[Mo] have the same geometry as Cu/NaF/Mo but atoms in the square brackets are absent. One can see that in the

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[Cu]/NaF/Mo case charge is more spread in the Z direction compared to the case when both Cu adatom and Mo support are removed ([Cu]/NaF/[Mo]). In particular, for [Cu]/NaF/Mo approximately 0.2 e are found above the position of Cu in Cu/AB/Mo (note, there is no Cu in [Cu]/NaF/Mo). The same conclusion follows from the cumulative magnetisation curve, which agrees well with the cumulative charge curve (Fig. S1).

2 Supplementary information to the subsection *Charge transfer from metal support to adatom through thin film: Cu/NaF/Mo case*

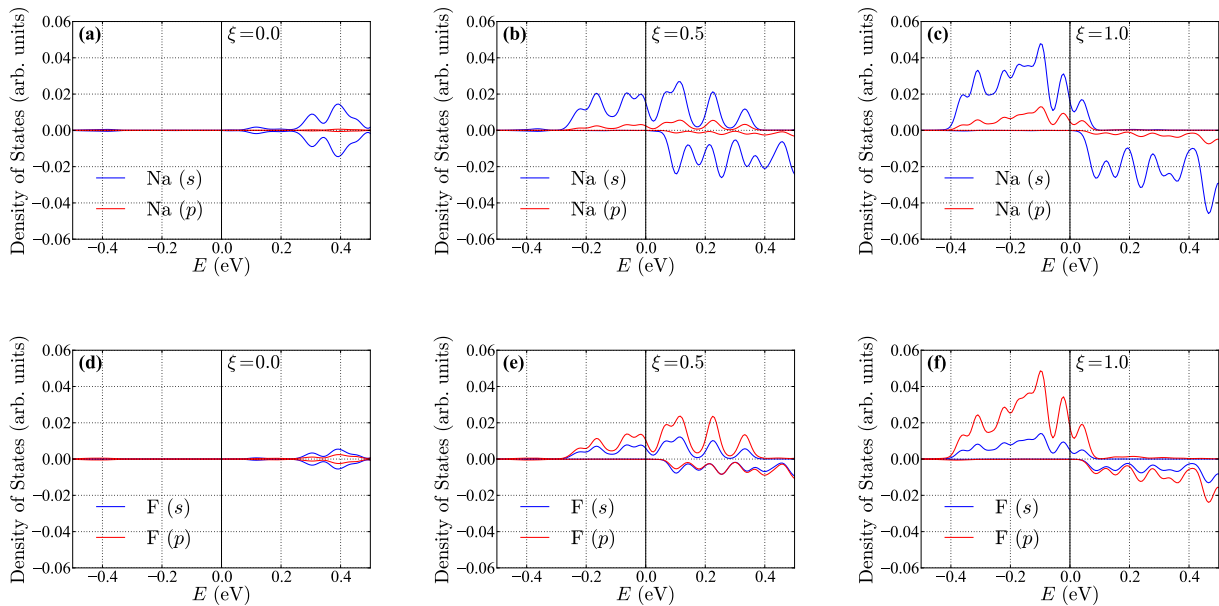


Figure S2: [Cu]/NaF/Mo partial density of states near the Fermi level (set to zero). (a), (b) and (c) Na atom (which is near Cu adatom in Cu/NaF/Mo). (d), (e) and (f) F atom (which is below Cu adatom in Cu/NaF/Mo). In (a) and (d) $\xi = 0.0$, in (b) and (e) $\xi = 0.5$, in (c) and (f) $\xi = 1.0$.

Here we report the details behind the distortion of [Cu]/NaF/Mo from $\xi = 0$ to $\xi = 1$. Fig. S2 shows the evolution of the density of states (DOS) near the Fermi level for [Cu]/NaF/Mo (F atom underneath Cu in Cu/NaF/Mo and the nearest Na atoms in the top NaF layer). The Bader charges of these atoms increase, while the charges of Mo atoms in the interface layer decrease, which agrees well with the evolution of DOS. The number of the F states below the Fermi level (mainly $2p_z$) and Na states (mainly $3s$) gradually increases along the deformation path, while the number of the Mo states decreases (not shown). Due to the charge transfer the system becomes spin polarised. Altogether this indicates that the F $2p$ and Na $3s$ states participate in the charge transfer to Cu adatom.