Supporting Information

Moisture effect on the diffusion of Cu ions in Cu/Ta$_2$O$_5$/Pt and Cu/SiO$_2$/Pt resistance switches: a first-principles study

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**Figure S1**: The stable structures and corresponding adsorption energies for the adsorption of a single H$_2$O on pure a-Ta$_2$O$_5$ surface. To obtain these structures, all the possible adsorption sites, including on the top of Ta or O atom on the a-Ta$_2$O$_5$ surface, have been considered.

(1) $E_{ads} = -1.02$ eV
(2) $E_{ads} = -0.74$ eV
(3) $E_{ads} = -0.97$ eV
(4) $E_{ads} = -1.61$ eV
(5) $E_{ads} = -0.71$ eV
(6) $E_{ads} = -0.68$ eV
(7) $E_{ads} = -0.50$ eV
(8) $E_{ads} = -1.30$ eV
**Figure S2:** The stable structures and corresponding adsorption energies for the adsorption of a single H$_2$O on pure a-SiO$_2$ surface. To obtain these structures, all the possible adsorption sites, including on the top of Si or O atom on the a-SiO$_2$ surface, have been considered.

1. $E_{\text{ads}} = -0.91$ eV
2. $E_{\text{ads}} = -0.43$ eV
3. $E_{\text{ads}} = -0.38$ eV
4. $E_{\text{ads}} = -0.36$ eV
5. $E_{\text{ads}} = -0.33$ eV
6. $E_{\text{ads}} = -0.31$ eV
7. $E_{\text{ads}} = -0.18$ eV
8. $E_{\text{ads}} = -0.18$ eV
9. $E_{\text{ads}} = -0.11$ eV
Figure S3: The structures and corresponding adsorption energies for the adsorption of Cu on pure a-Ta₂O₅ surface

(1) $E_{\text{ads}} = -2.89$ eV
(2) $E_{\text{ads}} = -2.88$ eV
(3) $E_{\text{ads}} = -2.24$ eV

(4) $E_{\text{ads}} = -2.14$ eV
(5) $E_{\text{ads}} = -2.15$ eV
(6) $E_{\text{ads}} = -2.06$ eV

(7) $E_{\text{ads}} = -2.05$ eV
(8) $E_{\text{ads}} = -2.30$ eV
(9) $E_{\text{ads}} = -1.85$ eV
Figure S3 (continued): The structures and corresponding adsorption energies for the adsorption of Cu on pure α-Ta2O5 surface

(10) $E_{\text{ads}} = -1.70 \text{ eV}$

(11) $E_{\text{ads}} = -1.39 \text{ eV}$

(12) $E_{\text{ads}} = -1.16 \text{ eV}$

(13) $E_{\text{ads}} = -0.88 \text{ eV}$

(14) $E_{\text{ads}} = -0.65 \text{ eV}$
Figure S4: The structures and corresponding adsorption energies for the adsorption of Cu on α-Ta2O5-H2O surface

(1) $E_{ads} = -1.45 \text{ eV}$  
(2) $E_{ads} = -1.43 \text{ eV}$  
(3) $E_{ads} = -1.19 \text{ eV}$

(4) $E_{ads} = -0.96 \text{ eV}$  
(5) $E_{ads} = -0.92 \text{ eV}$  
(6) $E_{ads} = -0.72 \text{ eV}$

(7) $E_{ads} = -0.55 \text{ eV}$  
(8) $E_{ads} = -0.52 \text{ eV}$  
(9) $E_{ads} = -0.46 \text{ eV}$
Figure S4 (continued): The structures and corresponding adsorption energies for the adsorption of Cu on α-Ta₂O₅-H₂O surface

(10) $E_{ads} = -0.41$ eV

(11) $E_{ads} = -0.39$ eV

(12) $E_{ads} = -0.37$ eV

(13) $E_{ads} = -0.34$ eV

(14) $E_{ads} = -0.27$ eV