Supporting Data

Dissociative adsorption of 2,3,7,8-TCDD on the surfaces of typical metal oxides: A first-principles density functional theory study

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The meta-stable configurations of the physisorption of the 2,3,7,8-TCDD molecule on the MgO surface

In this part, the meta-stable orientations for the physisorption of the 2,3,7,8-TCDD molecule, whose energy has been listed in Table 2, are plotted for reference.

Parallel adsorptions

Configuration 1, adsorption energy -0.20 eV, 0.09 eV lower than the most stable parallel configuration.

Configuration 2, adsorption energy -0.18 eV, 0.11 eV lower than the most stable parallel configuration.
Configuration 3, adsorption energy -0.17 eV, 0.12 eV lower than the most stable parallel configuration.
Vertical configurations with C-Cl bonds pointing down

Configuration 1, adsorption energy -0.10 eV, 0.07 eV lower than the most stable orientation with C-Cl bonds pointing down.

Configuration 2, adsorption energy -0.07 eV, 0.10 eV lower than the most stable orientation with C-Cl bonds pointing down.
Configuration 3, adsorption energy -0.03 eV, 0.14 eV lower than the most stable orientation with C-Cl bonds pointing down.

Configuration 4, adsorption energy -0.02 eV, 0.15 eV lower than the most stable orientation with C-Cl bonds pointing down.

Configuration 5, adsorption energy -0.01 eV, 0.16 eV lower than the most stable orientation with C-Cl bonds pointing down.
Vertical configurations with C-H bond pointing to the surface.

Configuration 1, adsorption energy -0.14 eV, 0.01 eV lower than the most stable orientation of this category.

Configuration 2, adsorption energy -0.10 eV, 0.05 eV lower than the most stable orientation of this category.
Configuration 3, adsorption energy -0.03 eV, 0.12 eV lower than the most stable orientation of this category.

Configuration 4, adsorption energy -0.01 eV, 0.14 eV lower than the most stable orientation of this category.