Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Data

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

Shuo Zhao[a], Xiaodong Ma[a,*], Qin Pang[a], Hongwen Sun[a], Guichang Wang[b,*]

[a]Key Laboratory of Environmental Pollution Process and Standard, Ministry of Education, Tianjin Key Laboratory of Environmental Remediation and Pollution Control, College of Environmental Science and Engineering, Nankai University, Tianjin 300071, China

[b]Department of Chemistry and the Center of Theoretical Chemistry Study, Nankai University, Tianjin, 300071, China

Corresponding author:

Xiaodong Ma

Fax: +86 22 23501117

E-mail: **maxd@nankai.edu.cn**

Guichang Wang

Fax: +86 22 23502458.

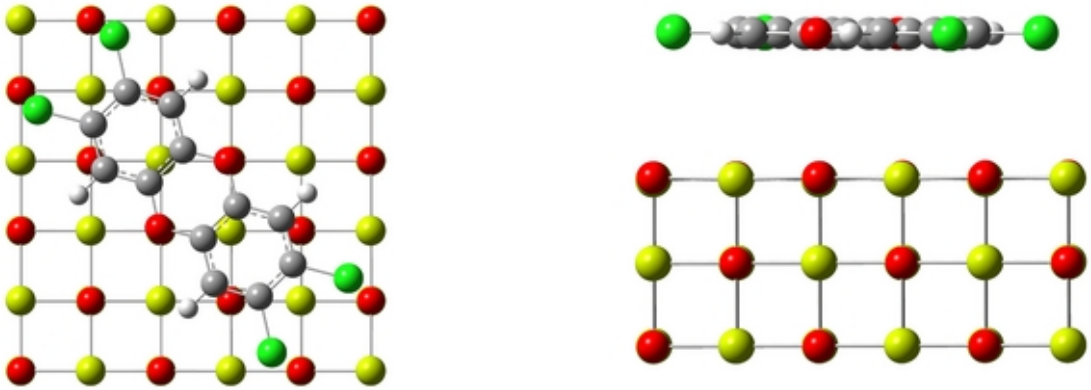
E-mail: wangguichang@nankai.edu.cn

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

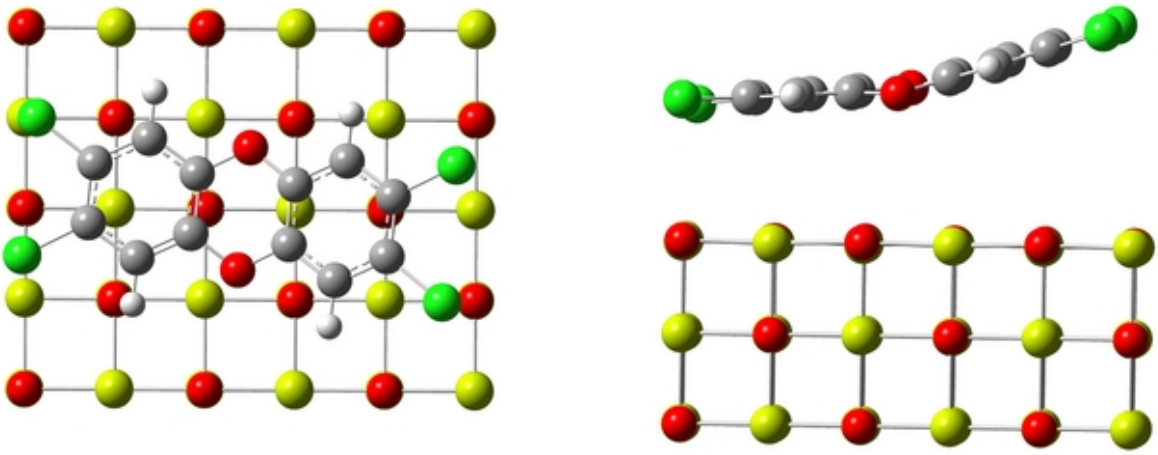
In this part, the meta-stable orientations for the physisorption of the 2,3,7,8-TCDD molecule, whose energy has been listed in Table 2, are plotted for reference.

Parallel adsorptions

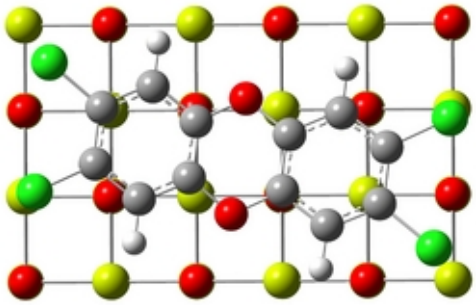
Configuration 1, adsorption energy -0.20 eV, 0.09 eV lower than the most stable parallel configuration.

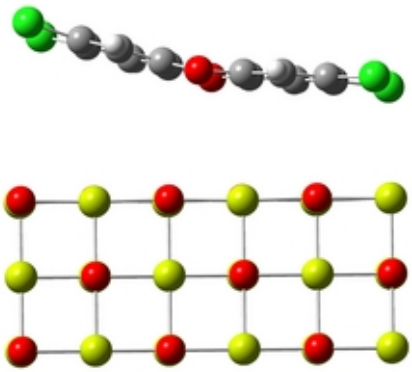


Configuration 2, adsorption energy -0.18 eV, 0.11 eV lower than the most stable parallel configuration.



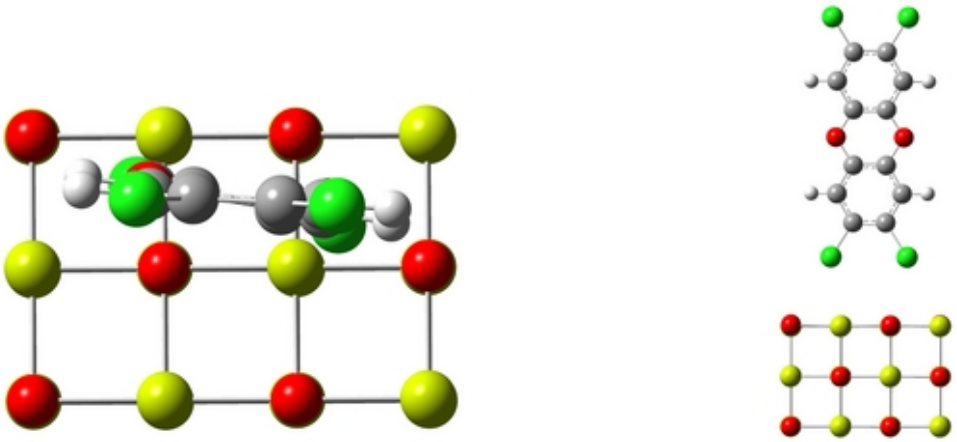
Configuration 3, adsorption energy -0.17 eV, 0.12 eV lower than the most stable parallel configuration.



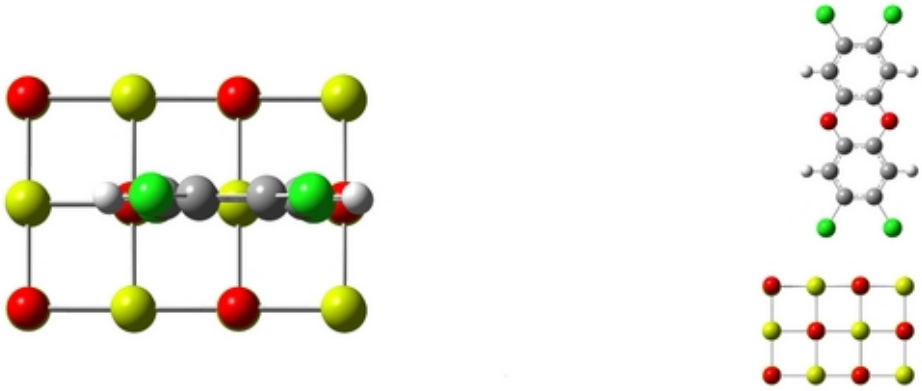


Vertical configurations with C-Cl bonds pointing down

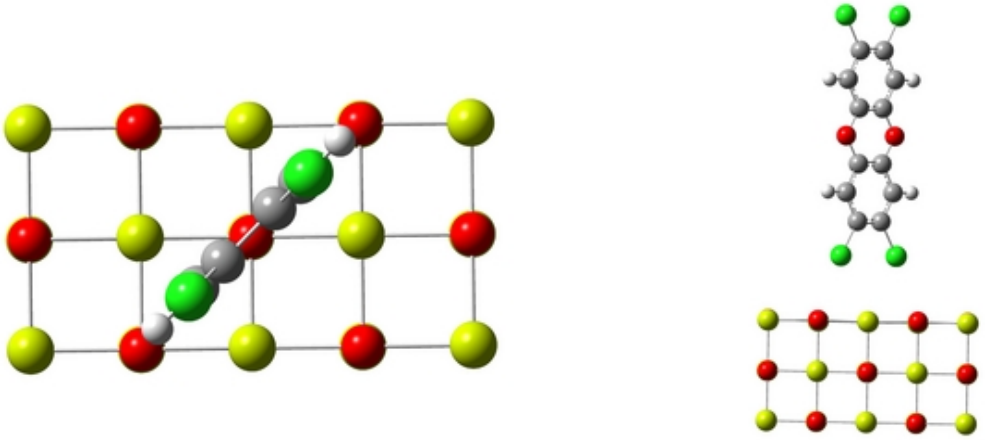
Configuration 1, adsorption energy -0.10 eV, 0.07 eV lower than the most stable orientation with C-Cl bonds pointing down.



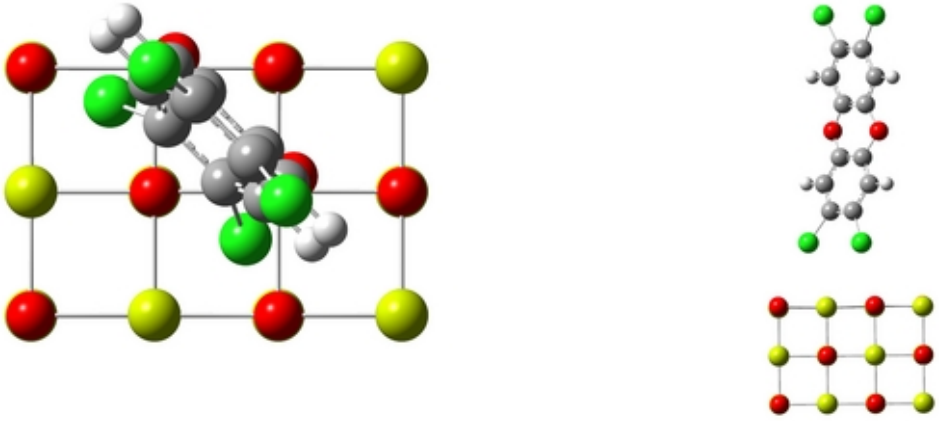
Configuration 2, adsorption energy -0.07 eV, 0.10 eV lower than the most stable orientation with C-Cl bonds pointing down.



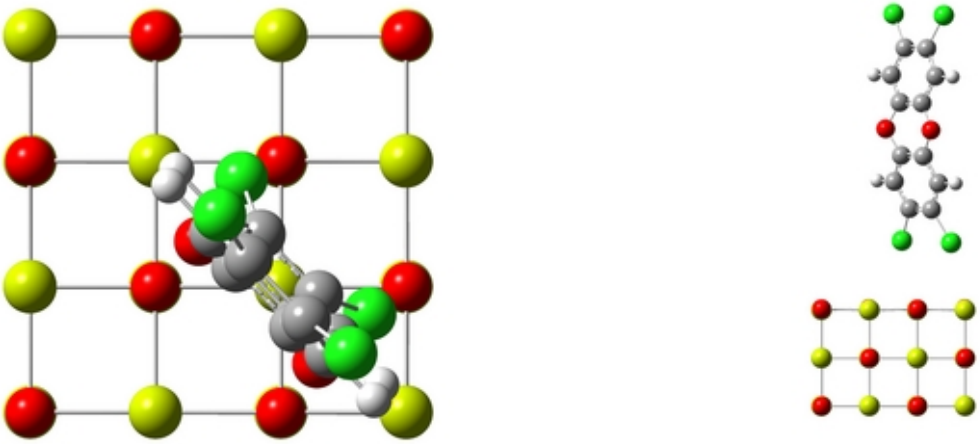
Configuration 3, adsorption energy -0.03 eV, 0.14 eV lower than the most stable orientation with C-Cl bonds pointing down.



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

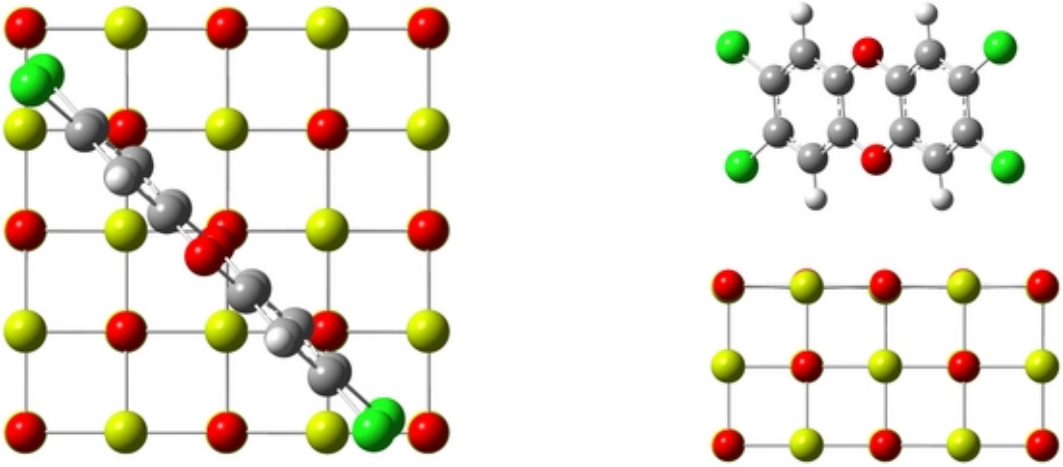


Configuration 5, adsorption energy -0.01 eV, 0.16 eV lower than the most stable orientation with C-Cl bonds pointing down.

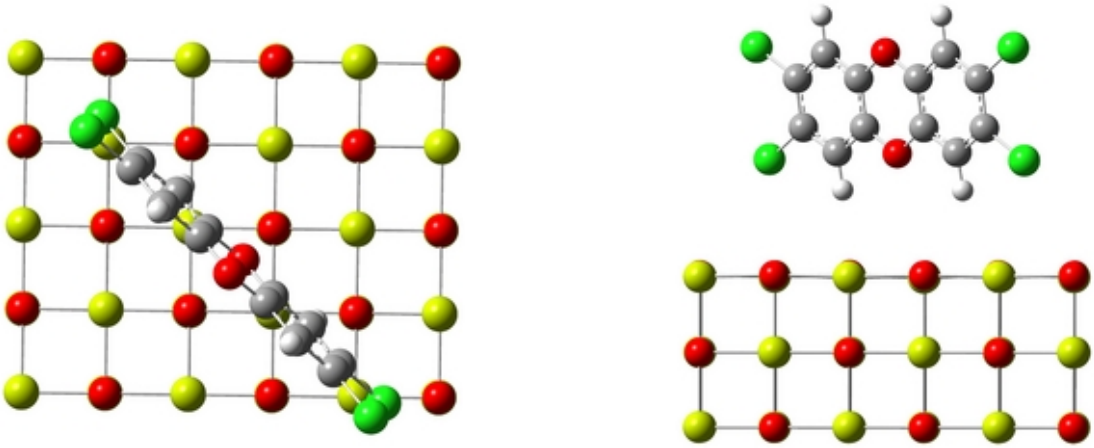


Vertical configurations with C-H bond pointing to the surface.

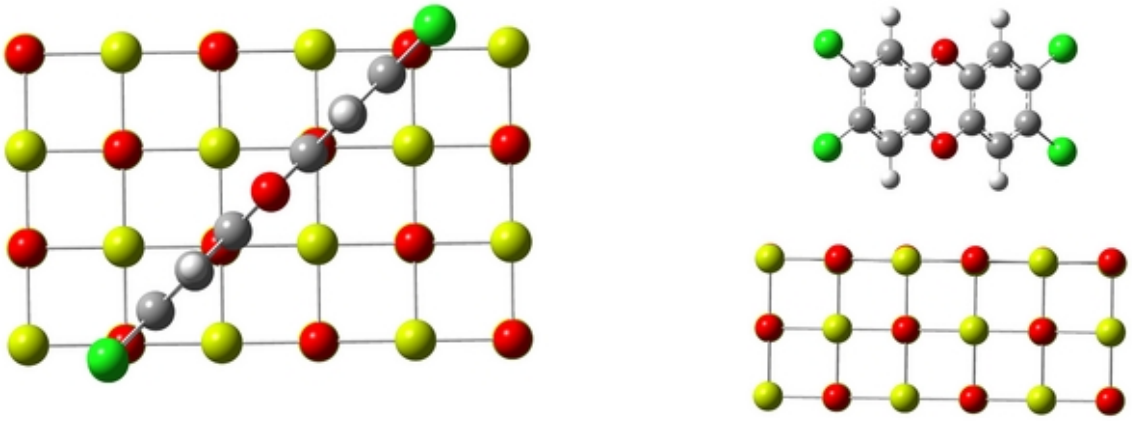
Configuration 1, adsorption energy -0.14 eV, 0.01 eV lower than the most stable orientation of this category.



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.