Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Adsorption of $[SiW_{12}O_{40}]^{4-}$ on the Ag(111) Surface: The IR Spectrum

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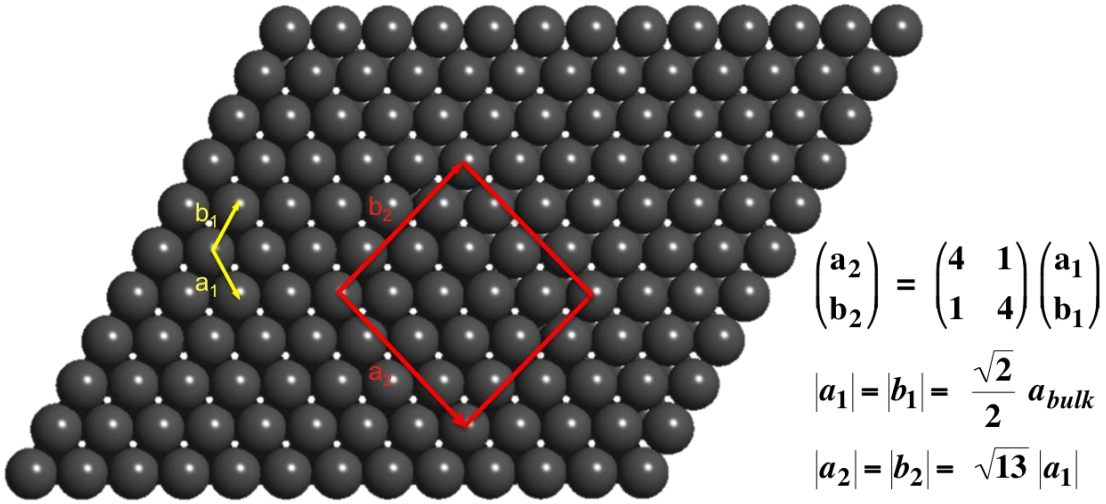
Figure S1. Adsorbate unit cell using matrix notation. The length of the surface unit cell vectors $\mathbf{a_1}$ and $\mathbf{b_1}$ is related to the bulk unit cell parameter, a_{bulk}. The Ag bulk parameter has been optimized at 4.15876 Å.[i] The length of the adsorbate unit cell vectors $\mathbf{a_2}$ and $\mathbf{b_2}$ is 10.6028 Å. The angle between vectors $\mathbf{a_2}$ and $\mathbf{b_2}$ is 92.9º (almost square unit cell). The angle between vectors $\mathbf{a_2}$ and $\mathbf{a_1}$ is 13.9º.



Vibrational normal modes visualization

Supporting information includes a set of .xyz files. Each file corresponds to different vibrational normal modes (VNM). The name of the files are the corresponding wavenumber associated with the VNM and, if it is necessary, the intensity of the band. The list of files is:

1011-11.xyz
1011-23.xyz
1002.xyz
1001.xyz
940.xyz
916.xyz
881.xyz

851.xyz
805.xyz
518.xyz
483.xyz
378.xyz
305.xyz
299.xyz
254.xyz

Each VNM can be visualized using "Jmol" code[ii]. With this open-source the VNM can be viewed as a set of static displacement vectors (select Vectors…) or/and as an animated mode (select Vibration).

References

[i] Martorell, B.; Clotet, A.; Fraxedas, J. A First Principle Study of the Structural, Vibrational and Electronic Properties of Tetrathiafulvalene Adsorbed on Ag(110) and Au(110) Surfaces. *J. Comput. Chem.* **2010** *31*, 1842-1852.

[ii] Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/