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ABSTRACT SYMPOSIUM NAME: Fundamental Insights in Catalytic Chemistry through Precisely Synthesized Materials: A Symposium Honoring Bruce C. Gates
ABSTRACT SYMPOSIUM PROGRAM AREA NAME: CATL
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TITLE: PTRF-XAFS investigation on the 3-dimensional structure of the single-atom metal dispersed on single crystal oxides
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ABSTRACT BODY:
Abstract: We have developed a PTRF-XAFS (polarization dependent total reflection fluorescence X-ray absorption fine structure) method which gives the 3-dimensional structure around the x-ray absorbing metal on single crystal oxide surfaces under ultra-high vacuum (UHV) conditions as shown in Fig.1[1] to investigate the structure of the single-atom metal species and the interaction between the support oxide and the metal species on single crystal oxides such as Al_2O_3(0001) and TiO_2(110). We have revealed the surface anions (oxygen atoms) not cations play a decisive role for the metal-oxide interaction and to determine the metal structure. The single-atom Ni or Cu can be formed on the oxide when two or more anions(oxygen atoms) are coordinated to the metal.[1] The modification of the surface by organic compounds with a S functional group which has strong interaction with Au can disperse Au atomically.[2] We have proposed the indicator to determine the single metal dispersion which is equal to the ratio of the bond dissociation energy of metal-metal bond and the bond dissociation energy sum of the metal-ligand bonds as shown in Figure 2.[3] The work provides a guideline to attain the highly dispersed single-atom catalyst on the oxide surface.
[1] Asakura, K. (2012). Vol. 24. Catalysis edited by J. J. Spivey & M. Gupta, pp. 281-322. Cambridge RSC publishing.
[2] Asakura, K., Takakusagi, S., et. al.(2013). Faraday Discussions 162, 165-177.
[3] Takakusagi, S. and Asakura, K., et.al.(2016). J.Phys,Chen, C. 120, 15785–15791.

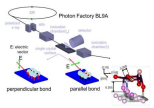

Figure 1 Schematics of PTRF-XAFS and single Ni atom on TiO_2(110)

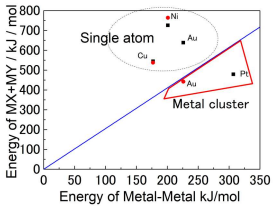

Figure 2 The formation energies of metal-metal and metal-O(S) and their relation to the atomic dispersions.