2.078 Molecular Insights into NO-Promoted Sulfate Formation on Model TiO2 Mineral Dust with Different Exposed Facets.

Early Career Scientist

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Abstract:

Industry exhaust (such as that from coal-fired plants)-initiated, sulfate aerosol formation on man-made mineral dust has not received a great deal of attention despite having a possible impact on the local environment. Titanium dioxide (TiO_2) nanoparticle is one of the most widely used materials in the purification of industrial exhaust. Nowadays, there is a lot of efforts, such as through morphology control, have been made to improve the performance of TiO_2 in the application, thus leading to unanticipated release of nano TiO_2 inside the operational areas or outsides the nearby atmosphere.

In this study, we choose the most available engineered TiO_2 nanomaterials with preferentially exposed (001), (010) and (101) facet as model oxides, to explore the possible reaction process and mechanism when they encounter NO and SO_2 under typical working conditions. DRIFTS spectra coupled with DFT calculations were used to investigate the dynamic adsorption behaviors of NO or/and SO_2 on the three facets while ion chromatography was adopted to quantify the surface products. Within the operational window of 100-400^oC insides the coal-fired plants, an obvious promotion effect of NO on the formation of sulfate species was found on all the faceted samples. Active oxygen species present in those low-coordinated surfaces play a determinant role in the promotion process, which enabled the oxidation of NO into NO_2. Then the adsorbed nitrate species resulting from the disproportionation of NO_2 dimer (N_2O_4) or gaseous NO_2 oxidize adsorbed sulfite into sulfate species. The T101, as the most stable facet existing in nano anatase TiO_2 dust with over 90% fraction, obtained the highest normalized amount of sulfate in the presence of NO. The occurrence of NO-promoted formation of sulfate under simulated atmospheric conditions (30^oC, 5 ppmv SO_2 and 10 ppmv NO) indicate that this promotion effect can be ubiquitous on well-engineered anthropogenic dusts.