Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Investigation of vanadia-alumina catalysts with solid-state NMR spectroscopy and DFT

Evgeniy Papulovskiy,*[a] Aleksandr A. Shubin,[ab] and Olga B. Lapina[a]

[a] Boreskov Institute of Catalysis, 630090 Novosibirsk, Russia.

[b] Novosibirsk State University, 630090 Novosibirsk, Russia

* e-mail: fyr@catalysis.ru

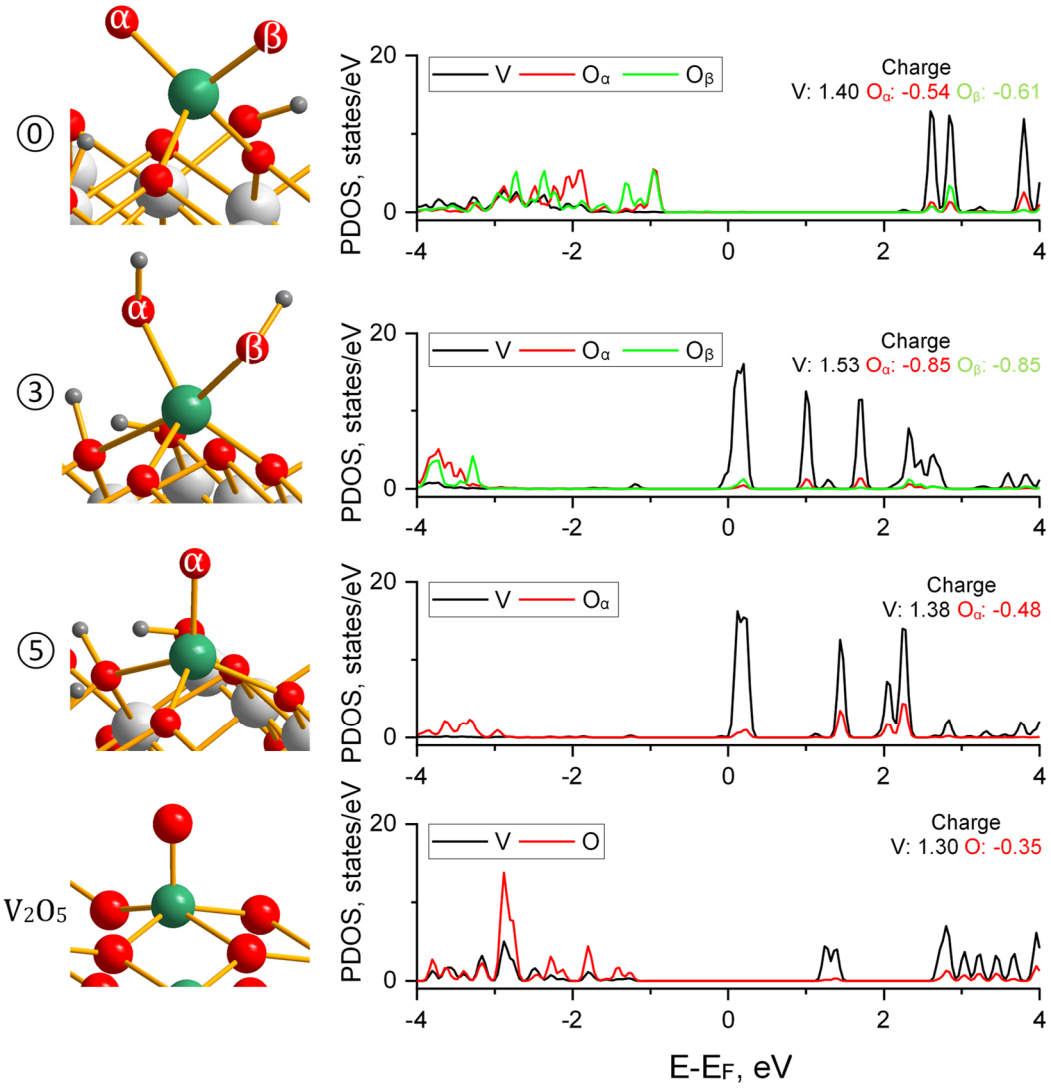

Figure S1. PDOS for the states of the site under investigation. The numbers to the left are referred to the reaction path, V_2O_5 is computed at the same level of theory to be used as a reference. Mulliken charges are also shown.