

Supplementary Materials: Removal Process of Structural Oxygen from Tetrahedrons in Muscovite during Acid Leaching of Vanadium-Bearing Shale

The climbing-image nudge elastic band (CI-NEB) method was employed for transition state (TS) search. We had inserted 5 images between the initial state and final state in the two pathway. The TS calculations were convergent when the total energy change and the forces on all unconstrained atoms were less than 10^{-5} eV and 0.05 eV/Å, respectively. The Figure S1 and Figure S2 show the reaction process of reverse-path and straight-path mechanisms, respectively. Only the reverse-path mechanism had search a transition state, then the frequency calculation of searched structure was carried out with all atoms fixed excluding the two hydroxyl. The vibrational frequencies of searched structure are listed in Table S1. The only one imaginary frequency (f/i) suggests that this structure exactly is a transition state.

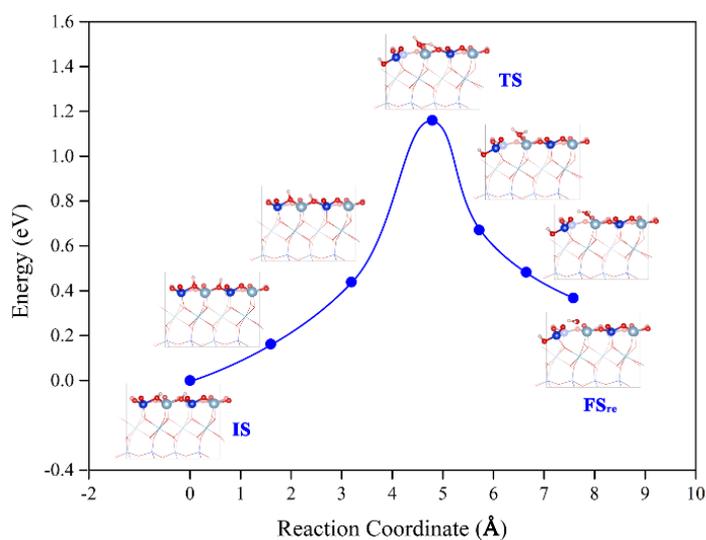


Figure S1. The reaction process of reverse-path mechanism.

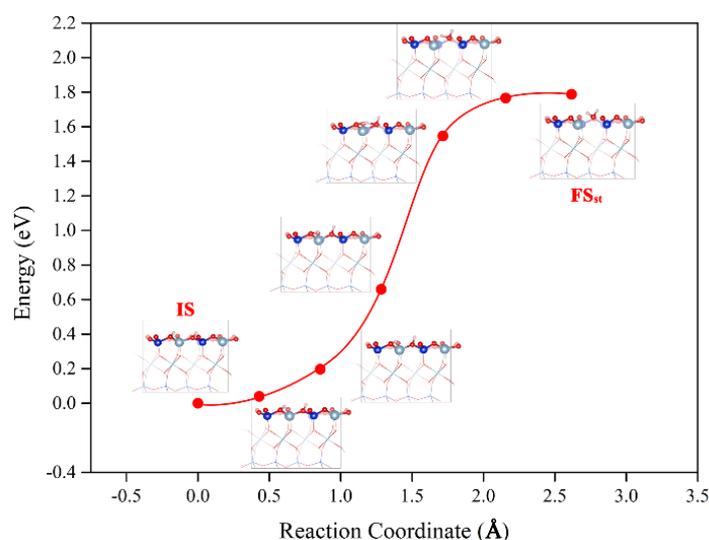


Figure S2. The reaction process of straight-path mechanism.

