Supplementary Information file for the manuscript:

Comparison of catalytic properties of vanadium centers introduced into BEA zeolite and present on (010) V_2O_5 surface – DFT studies

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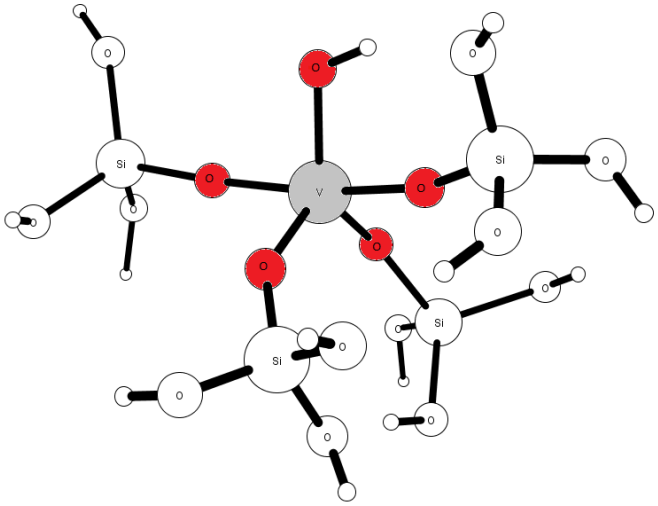
Small:



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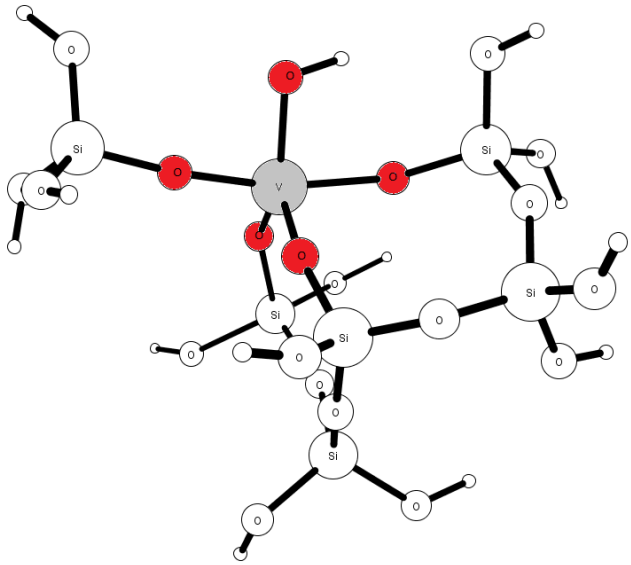

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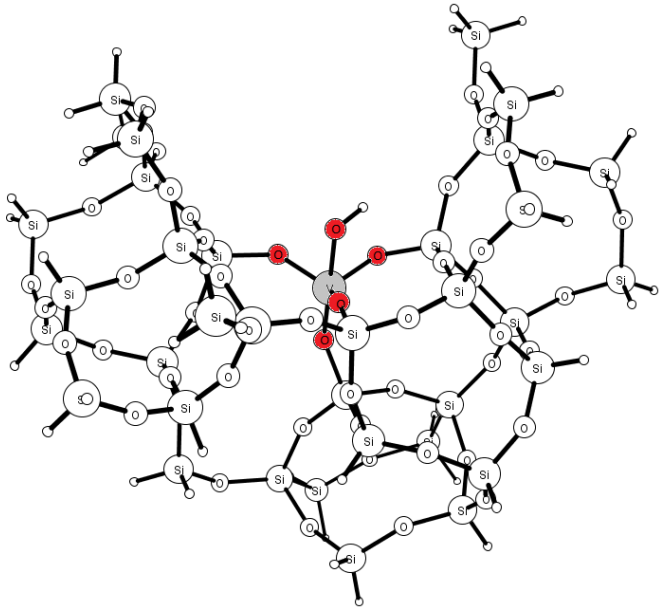

Figure S1. Clusters of various sizes representing the T3 center used to check the convergence of calculations.

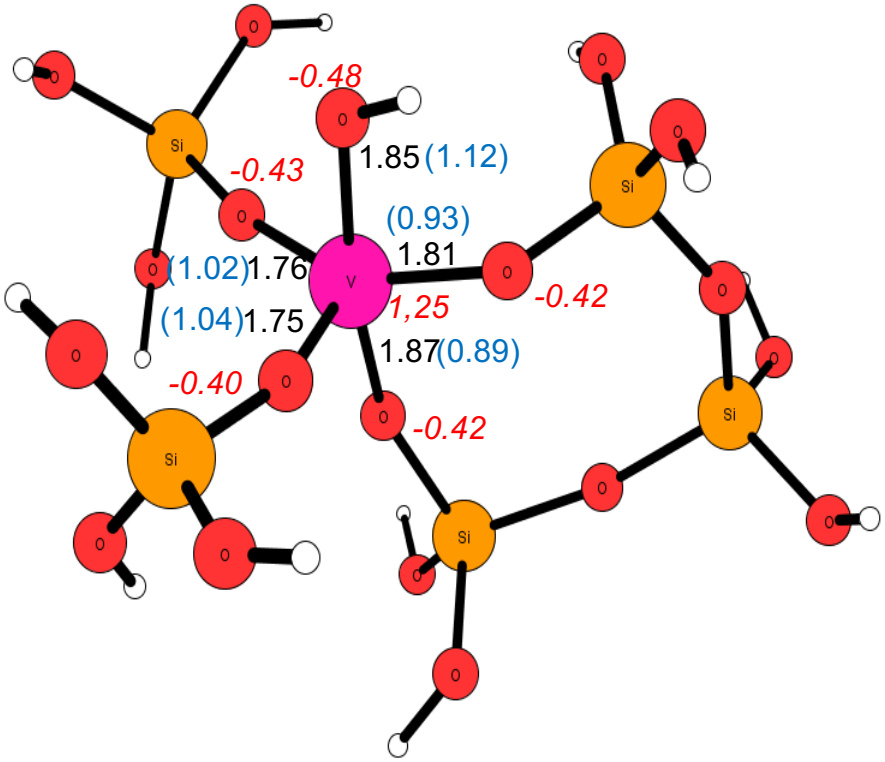

Figure S2. Computed parameters of V-OH center in T1 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

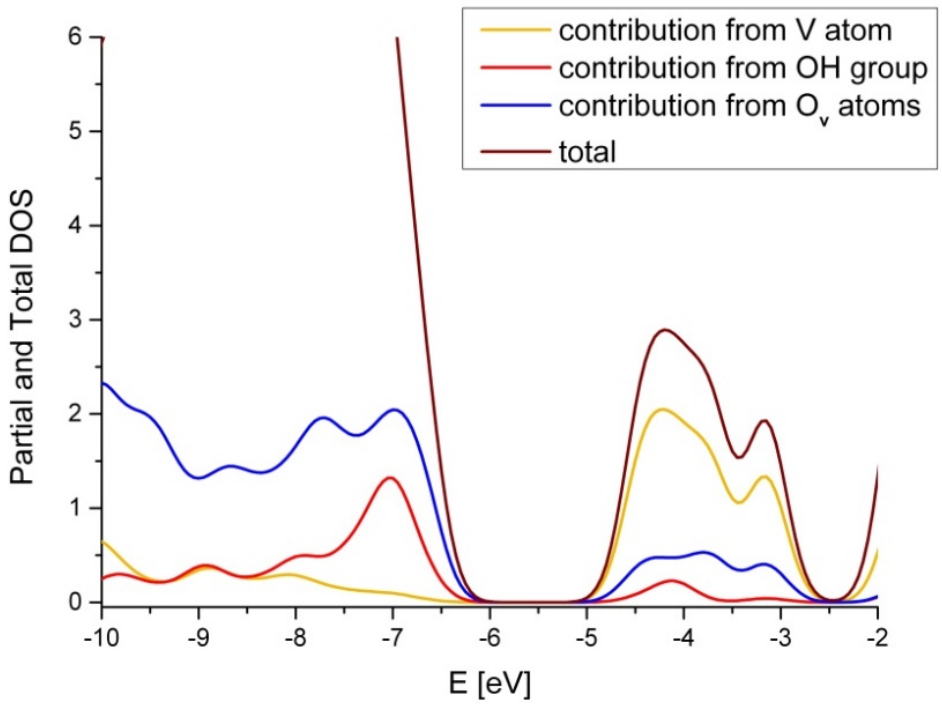

Figure S3. DOS plot for the system in which V-OH center is in T1 position.

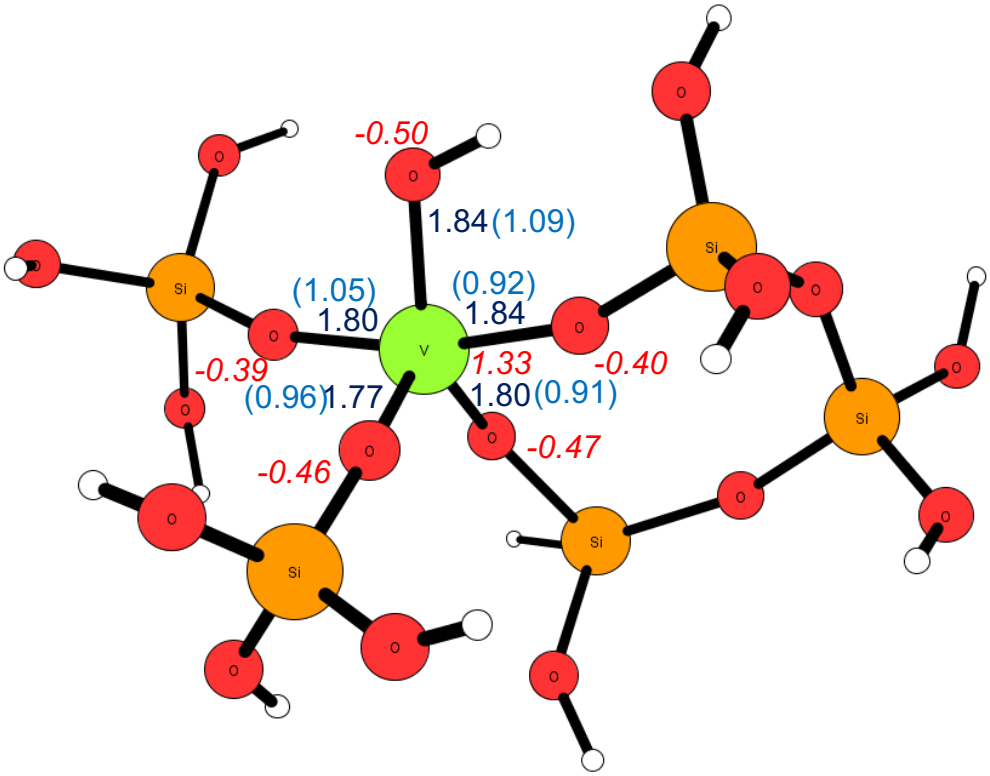

Figure S4. Computed parameters of V-OH center in T2 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

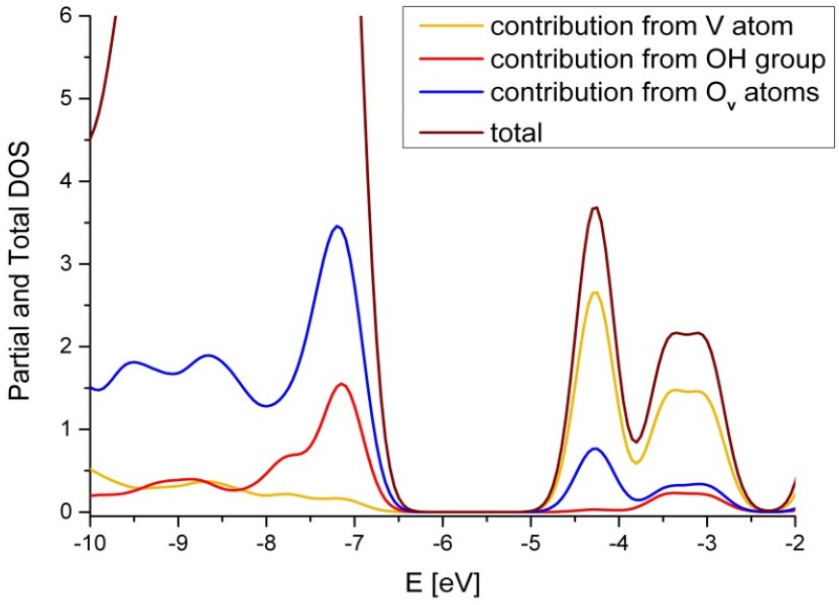

Figure S5. DOS plot for the system in which V-OH center is in T2 position.

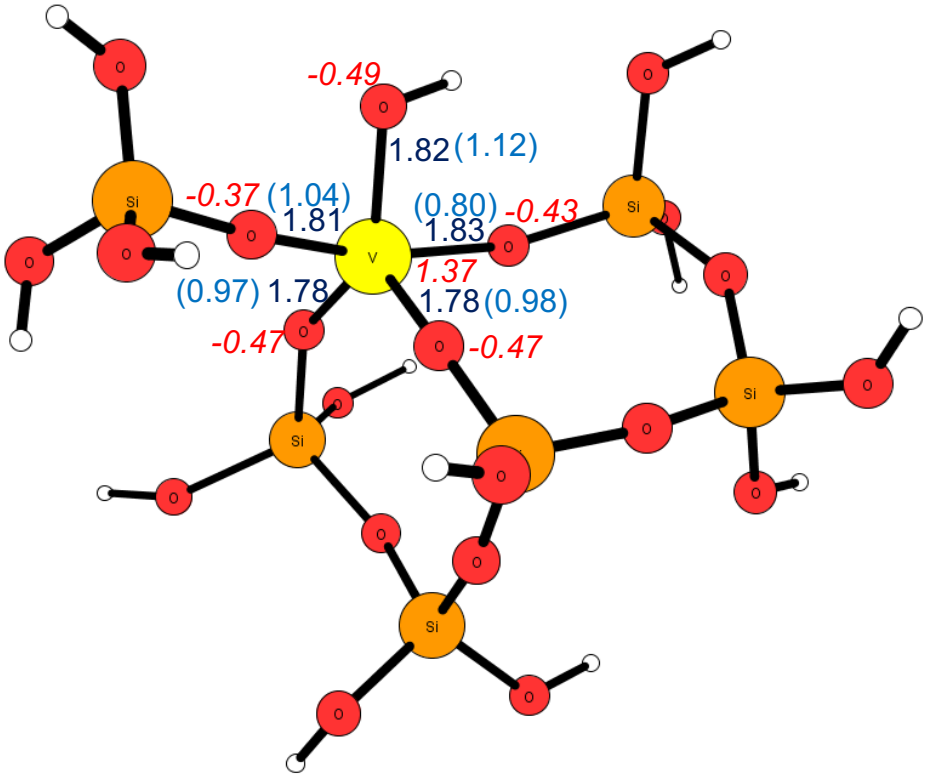

Figure S6. Computed parameters of V-OH center in T3 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

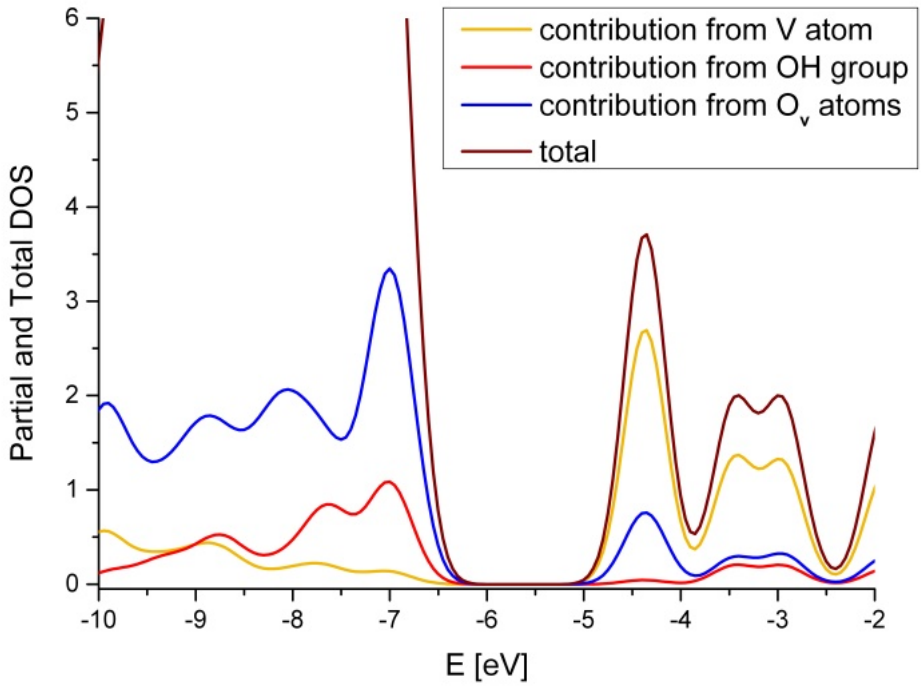

Figure S7. DOS plot for the system in which V-OH center is in T3 position.

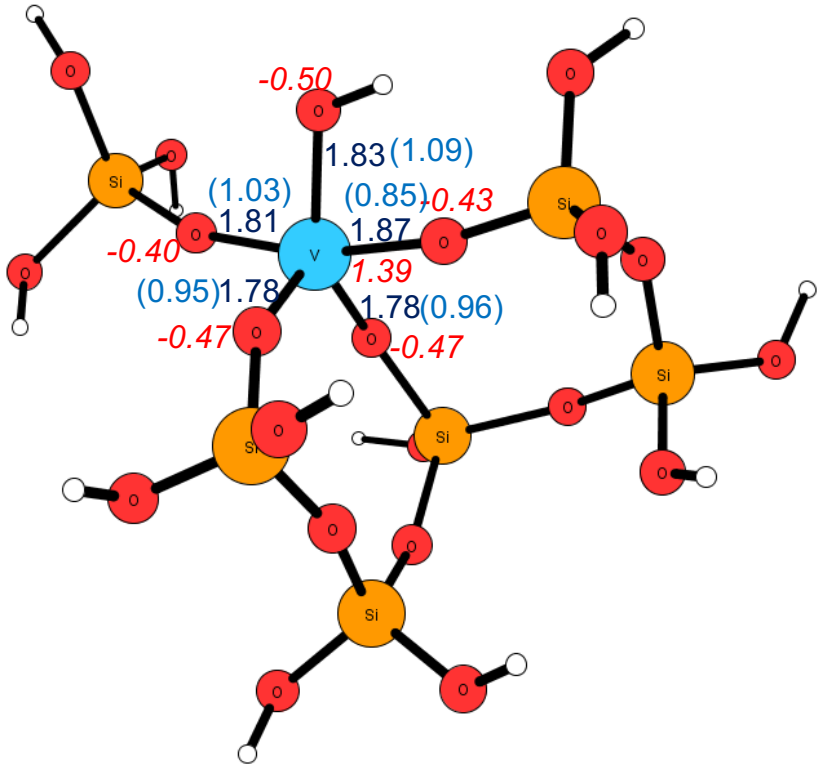

Figure S8. Computed parameters of V-OH center in T4 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

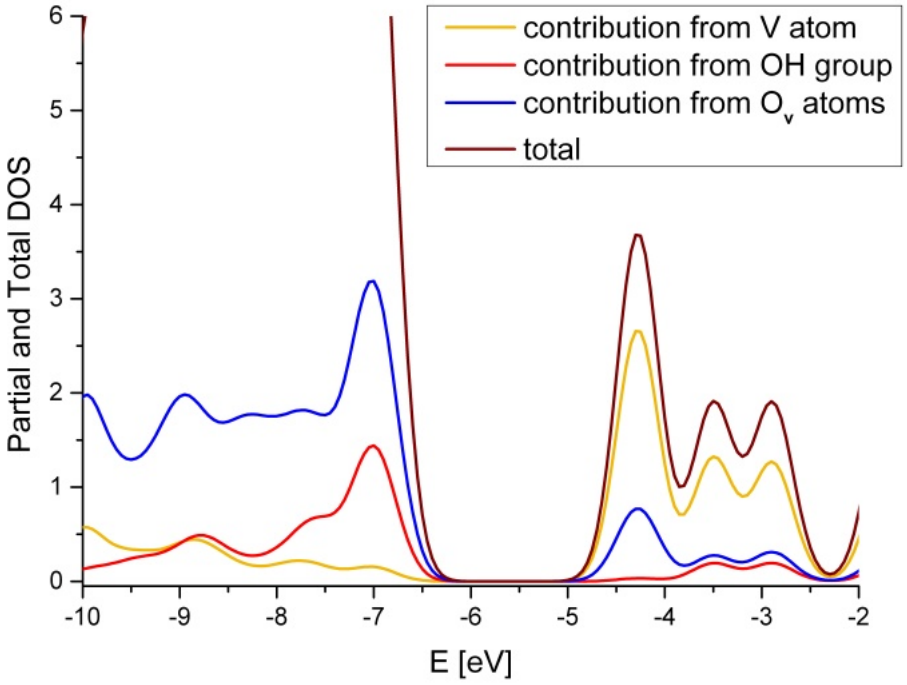

Figure S9. DOS plot for the system in which V-OH center is in T4 position.

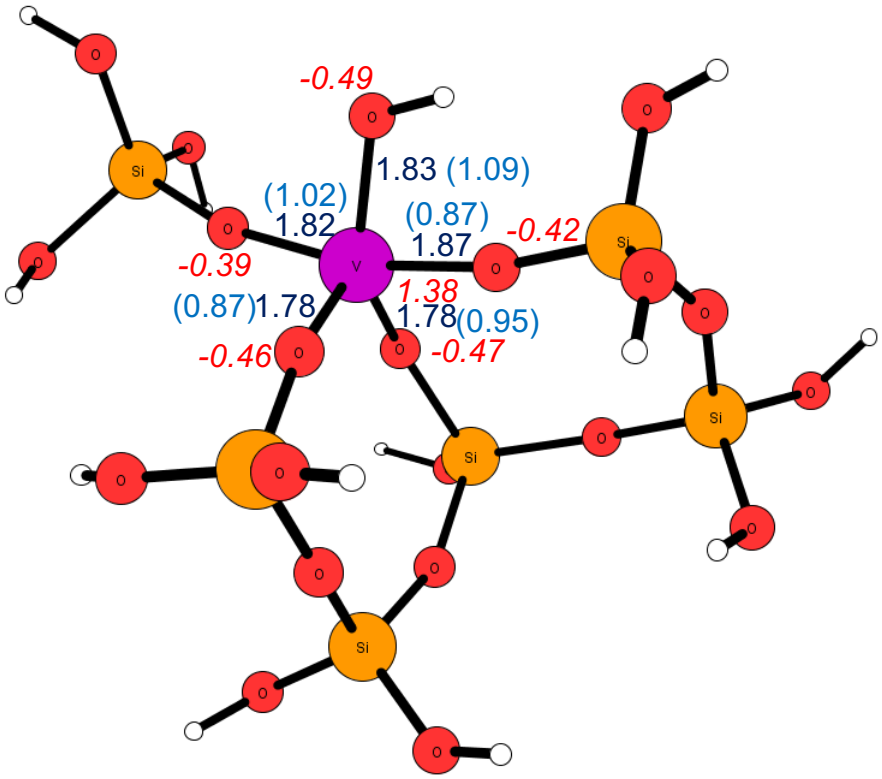

Figure S10. Computed parameters of V-OH center in T5 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

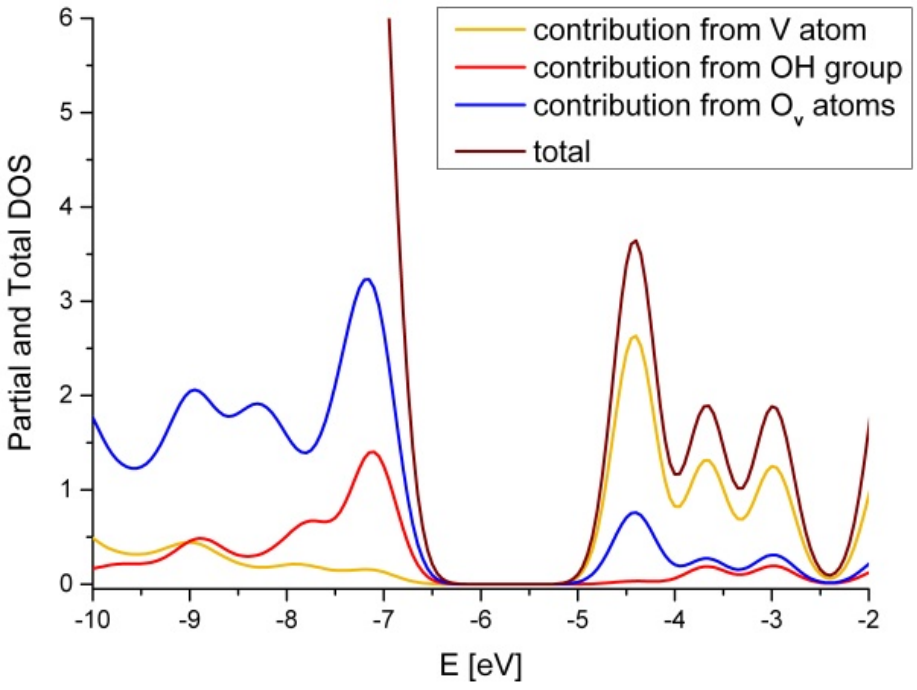

Figure S11. DOS plot for the system in which V-OH center is in T5 position.

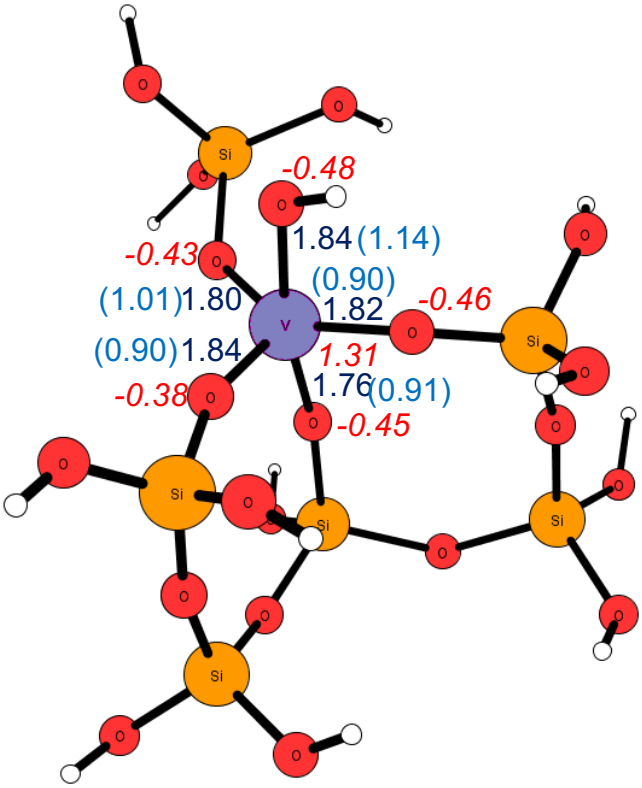

Figure S12. Computed parameters of V-OH center in T6 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

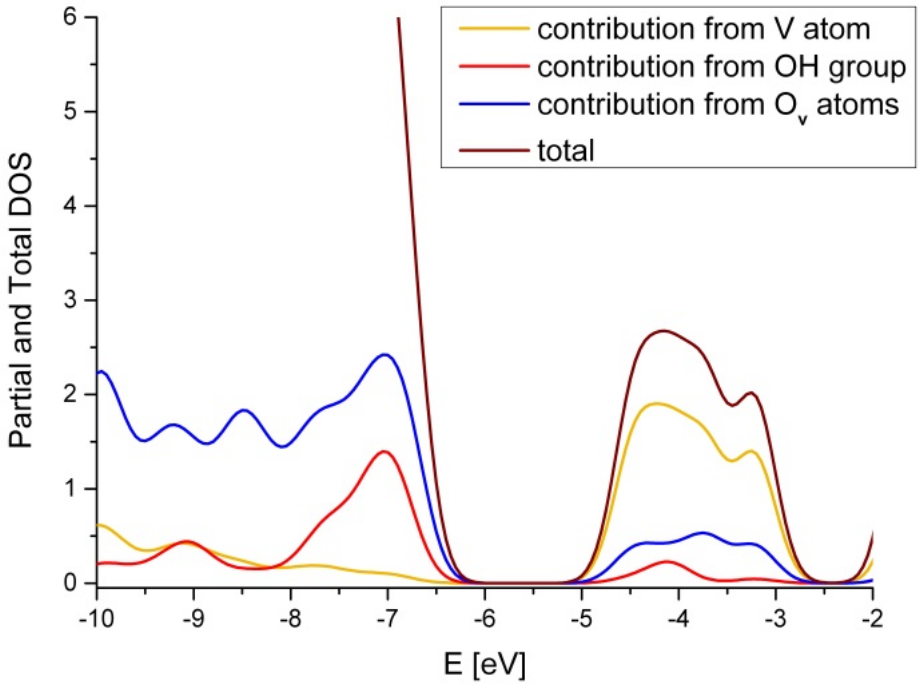

Figure S13. DOS plot for the system in which V-OH center is in T6 position.

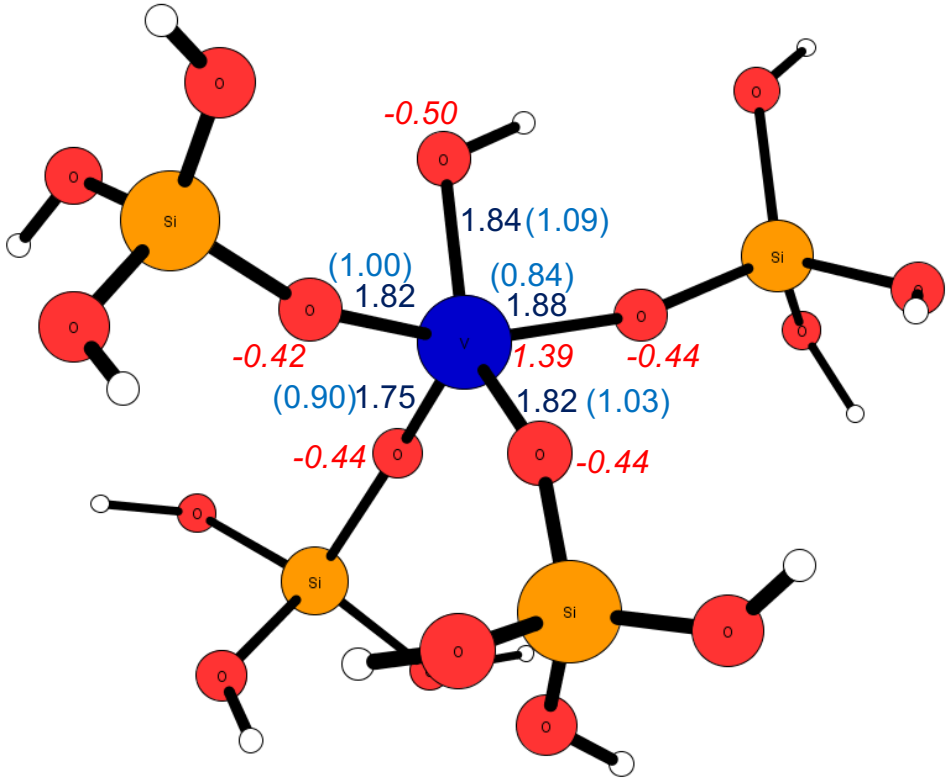

Figure S14. Computed parameters of V-OH center in T7 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

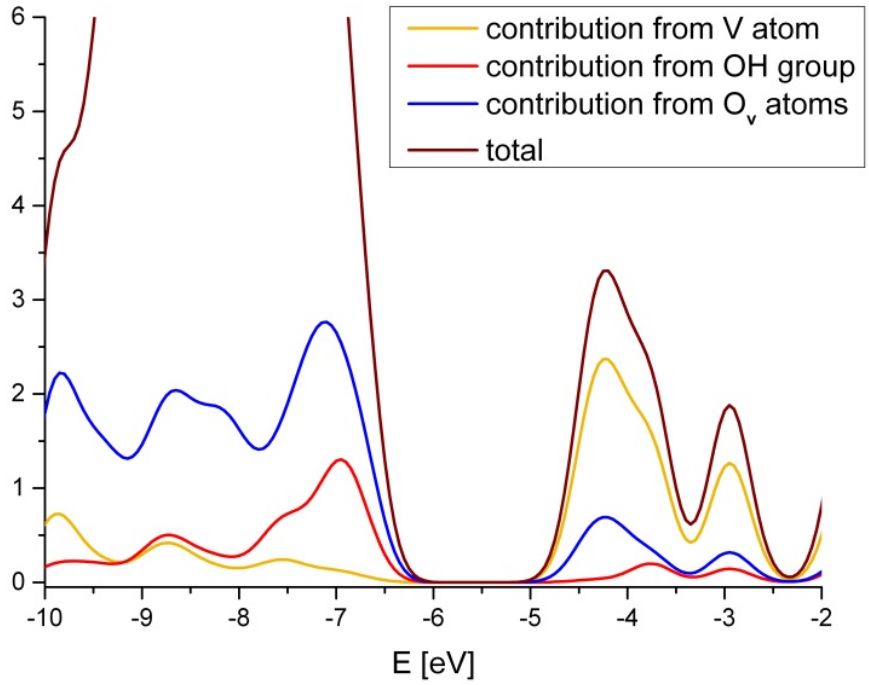

Figure S15. DOS plot for the system in which V-OH center is in T7 position.

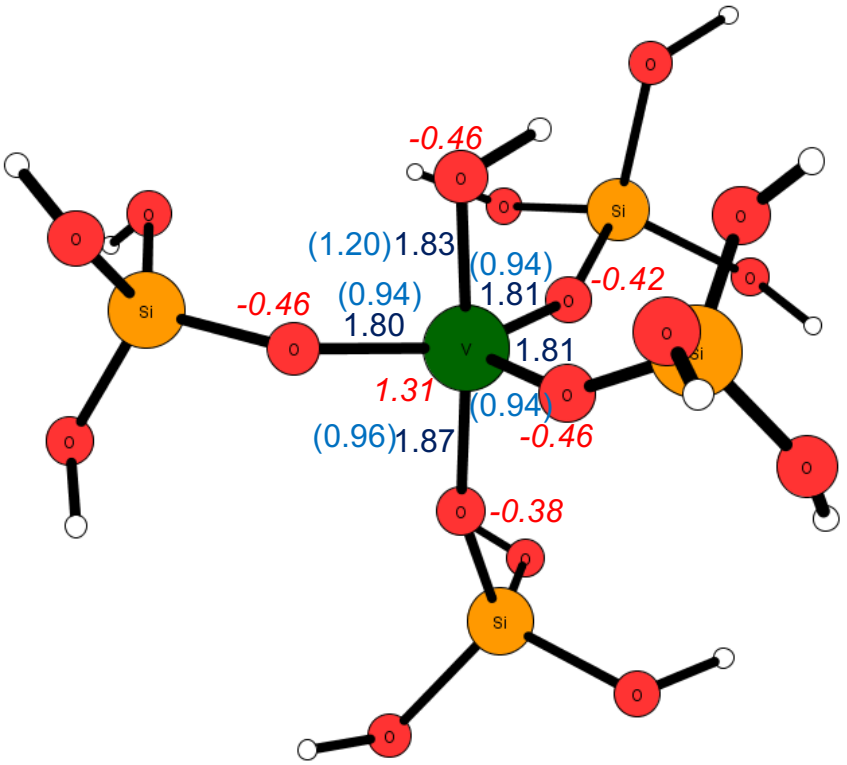

Figure S16. Computed parameters of V-OH center in T8 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

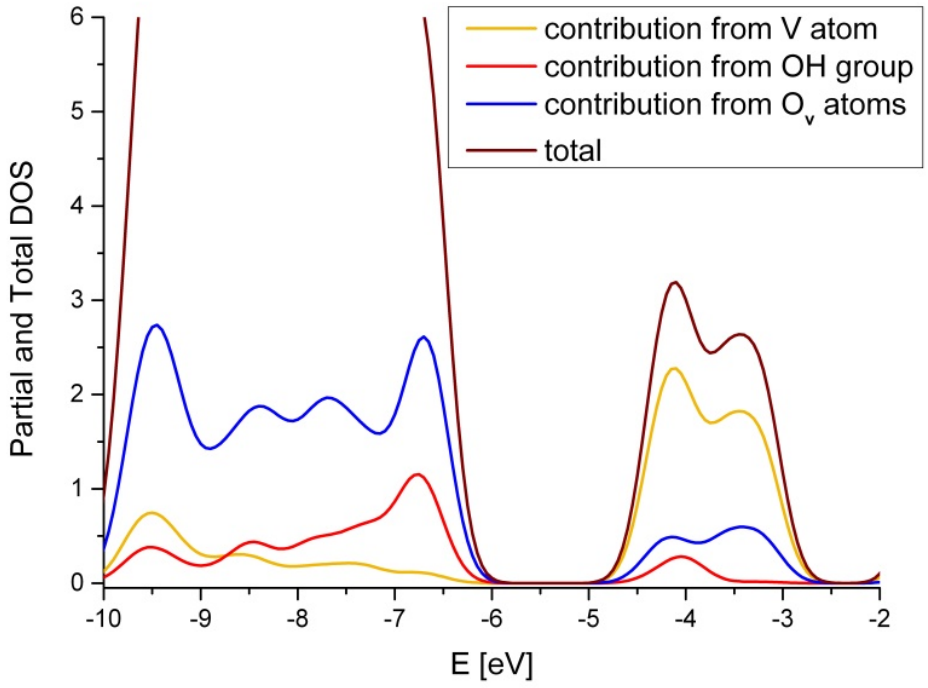

Figure S17. DOS plot for the system in which V-OH center is in T8 position.

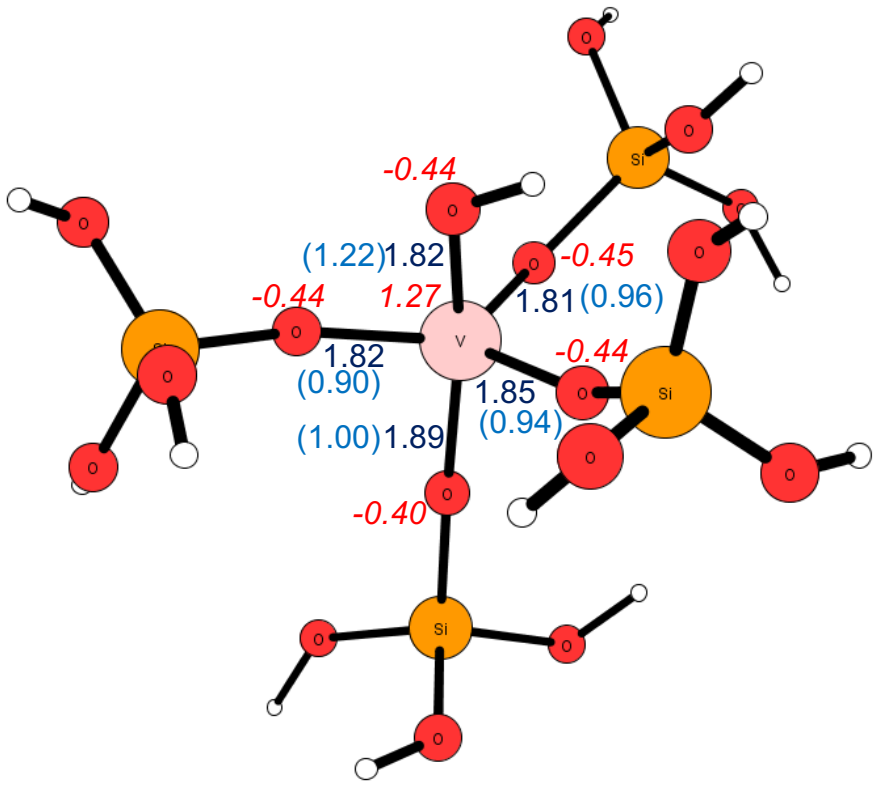

Figure S18. Computed parameters of V-OH center in T9 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

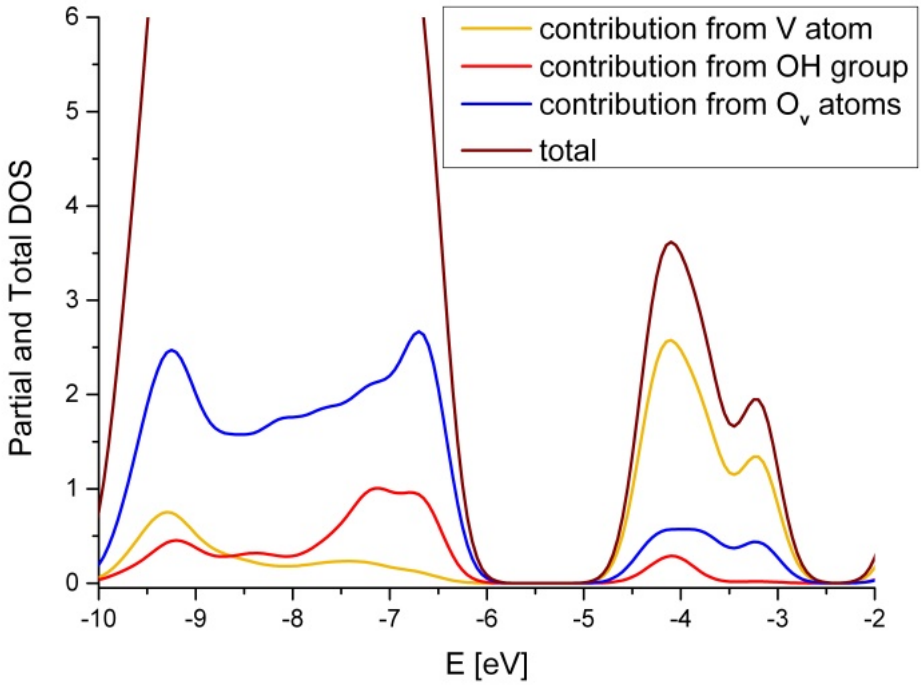

Figure S19. DOS plot for the system in which V-OH center is in T9 position.

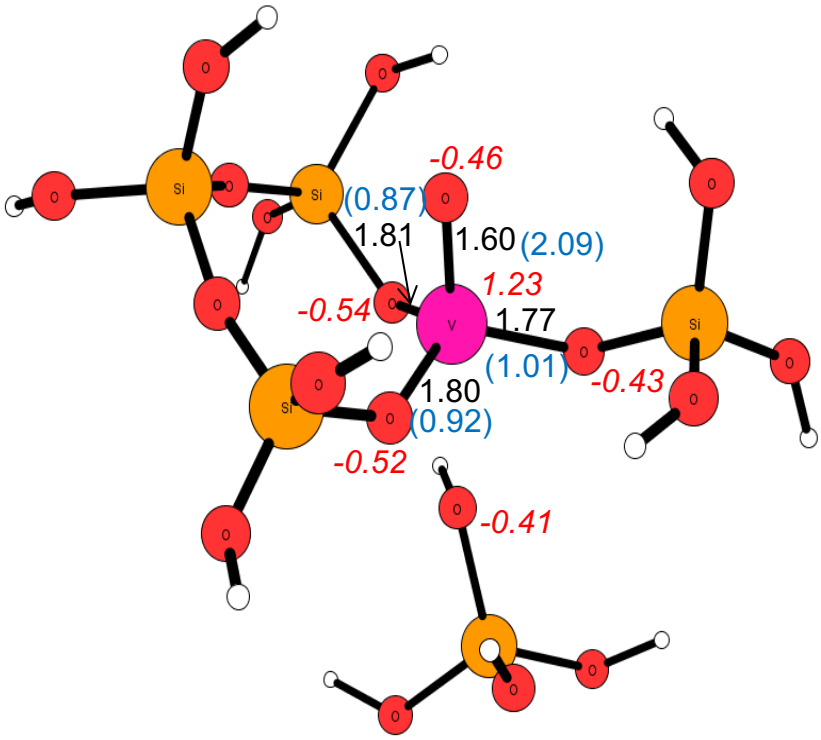

Figure S20. Computed parameters of V-O center in T1 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

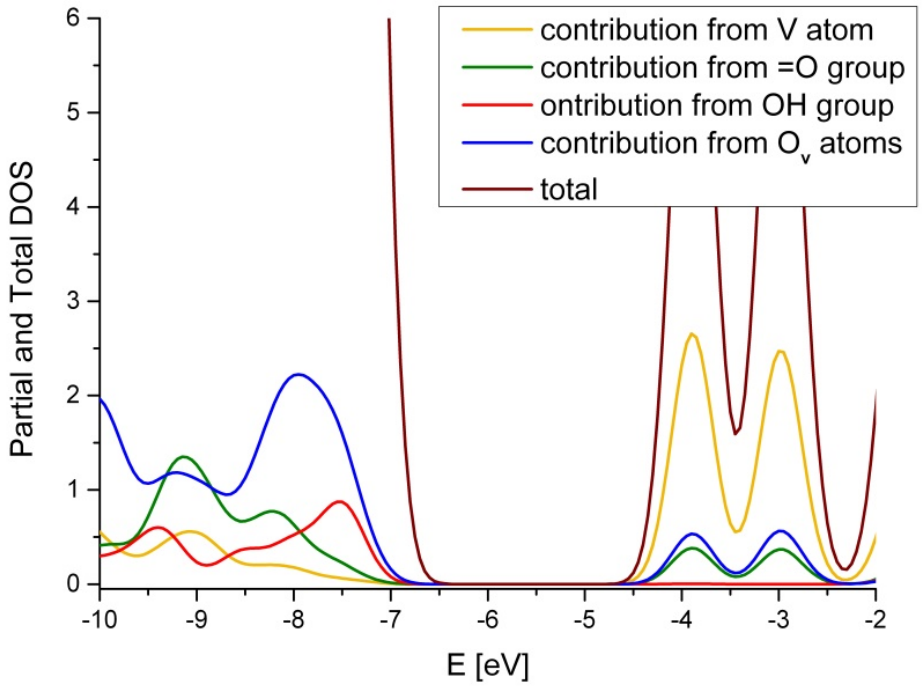

Figure S21. DOS plot for the system in which V-O center is in T1 position.

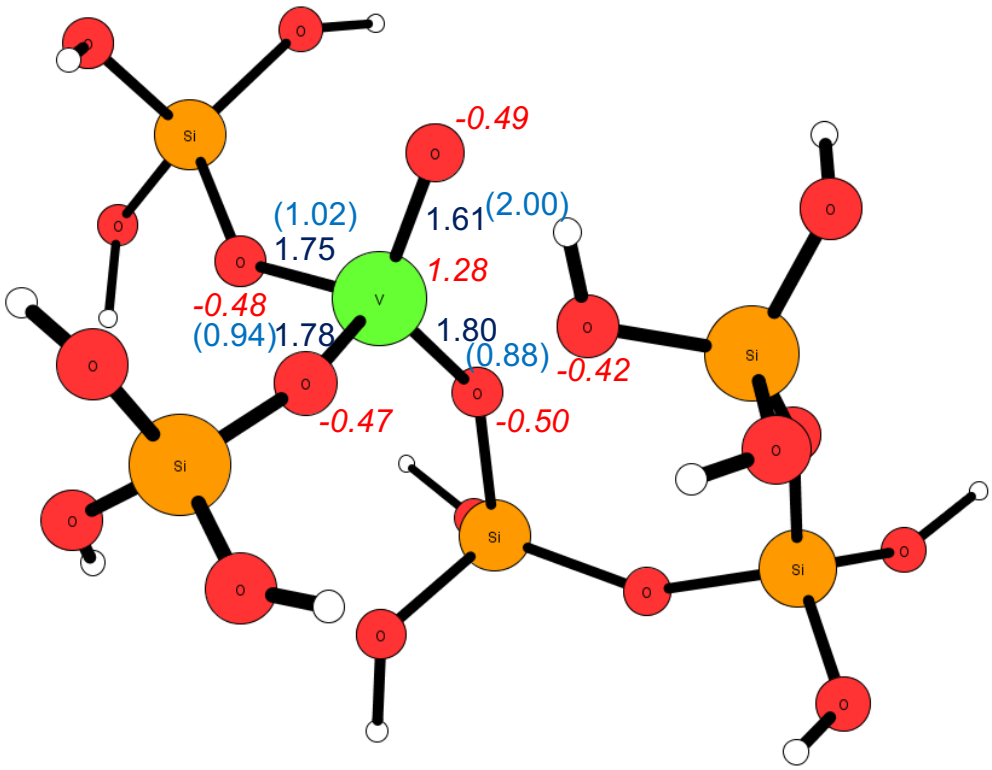

Figure S22. Computed parameters of V-O center in T2 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

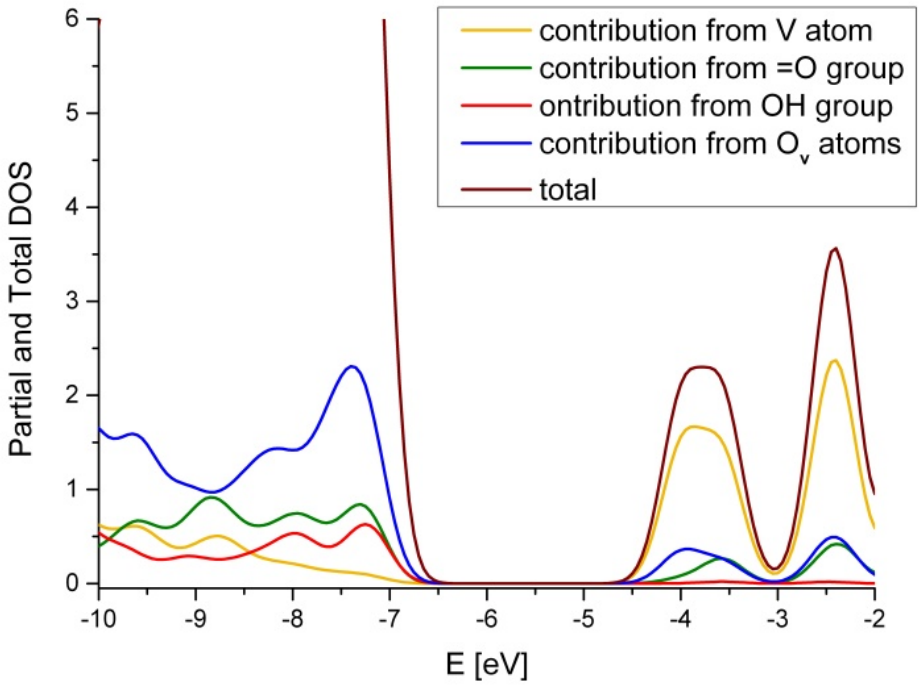

Figure S23. DOS plot for the system in which V-O center is in T2 position.

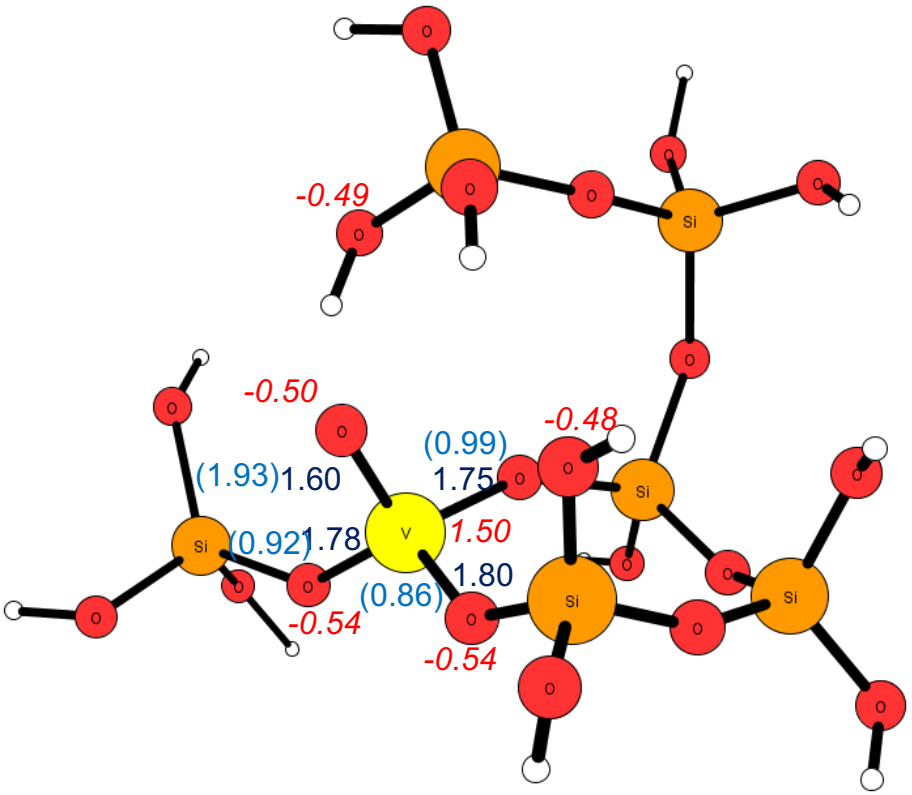

Figure S24. Computed parameters of V-O center in T3 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

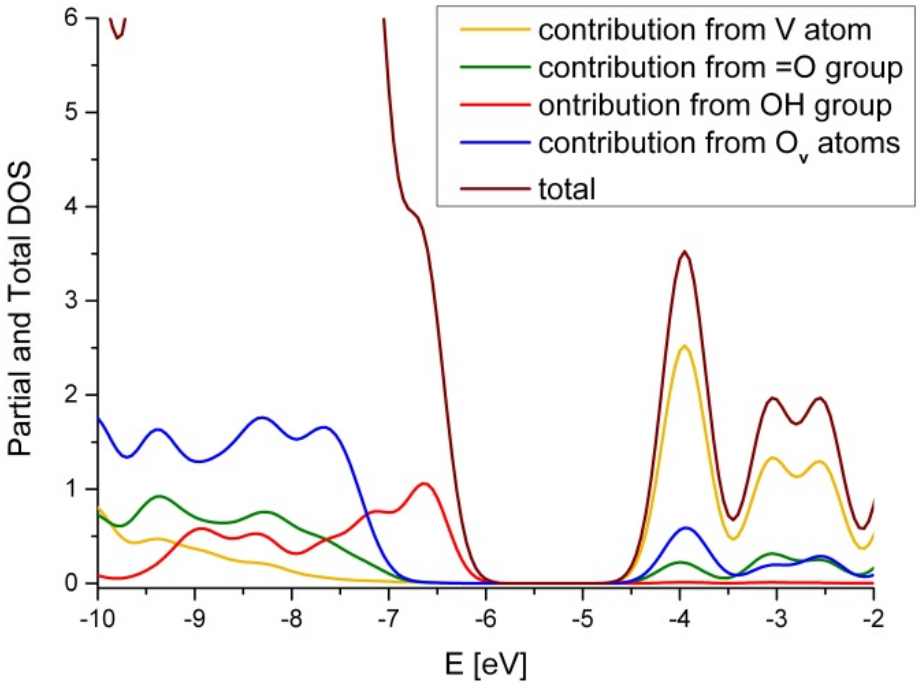

Figure S25. DOS plot for the system in which V-O center is in T3 position

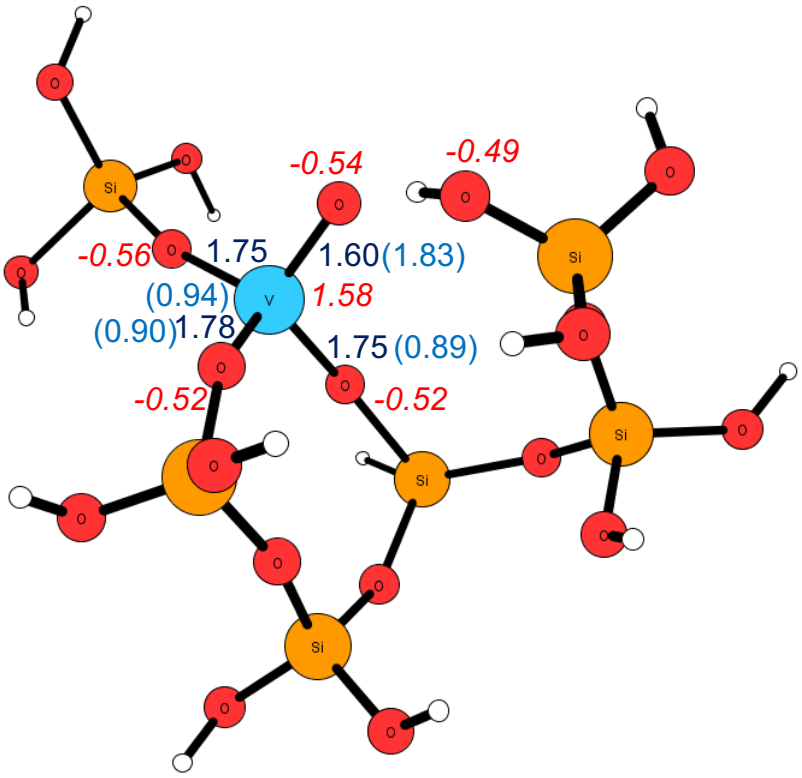

Figure S26. Computed parameters of V-O center in T4 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

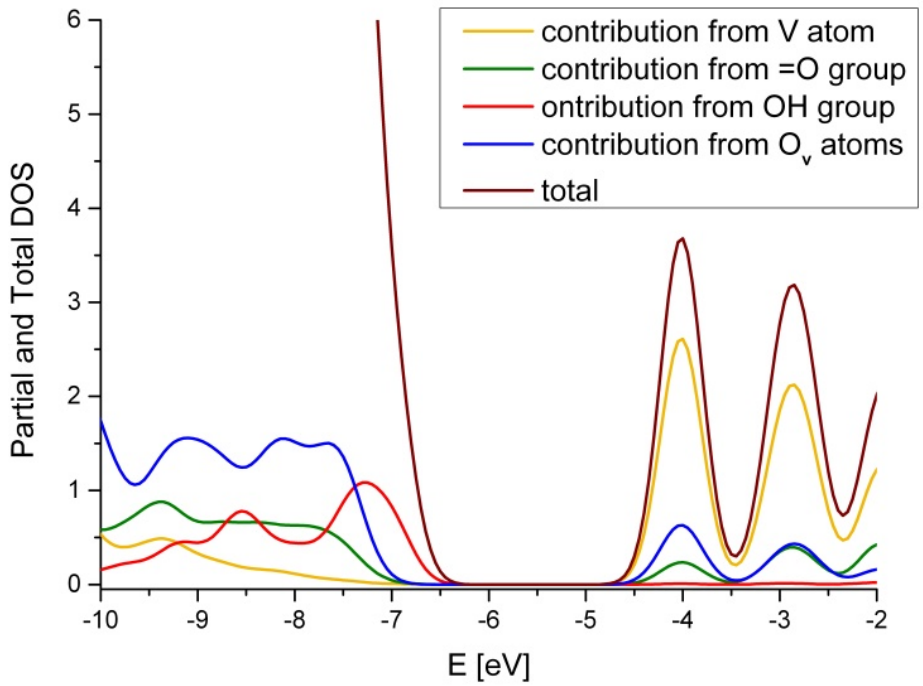

Figure S27. DOS plot for the system in which V-O center is in T4 position.

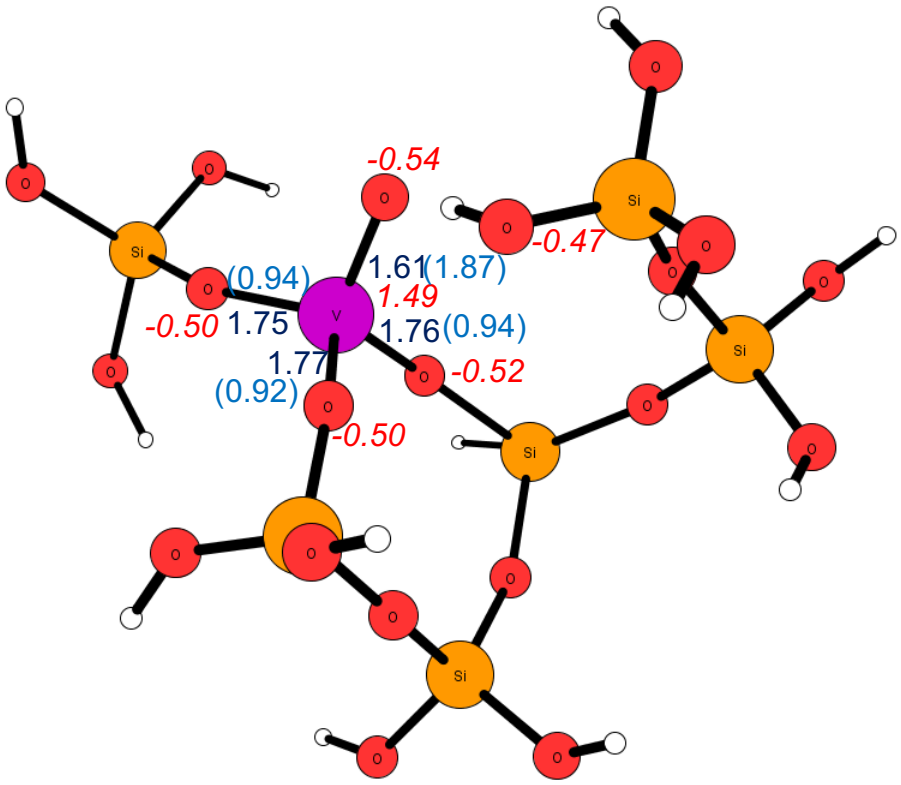

Figure S28. Computed parameters of V-O center in T5 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

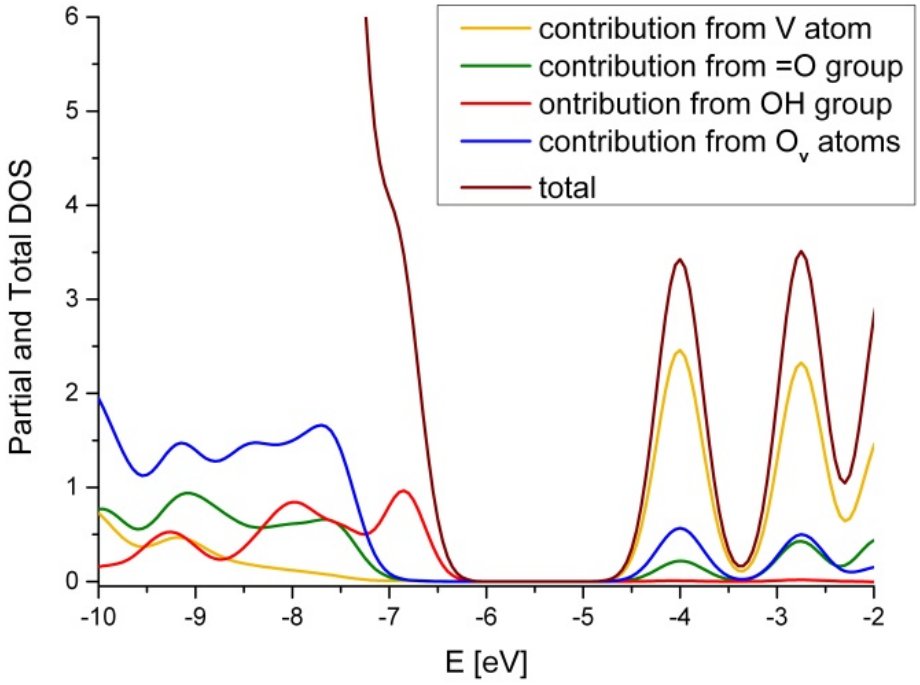

Figure S29. DOS plot for the system in which V-O center is in T5 position

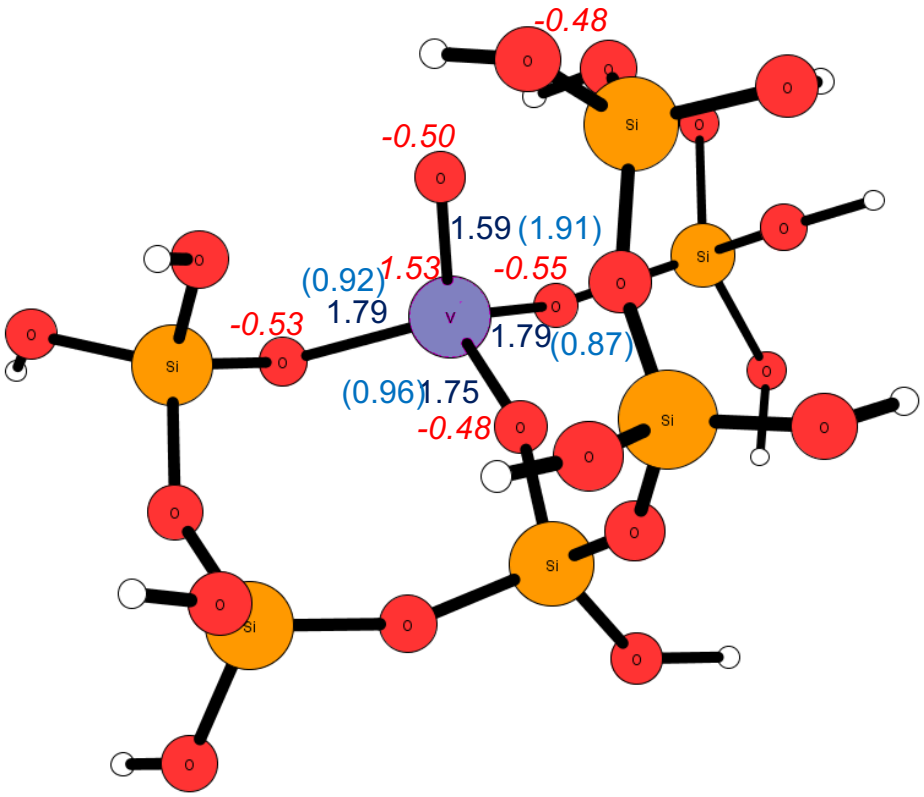

Figure S30. Computed parameters of V-O center in T6 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

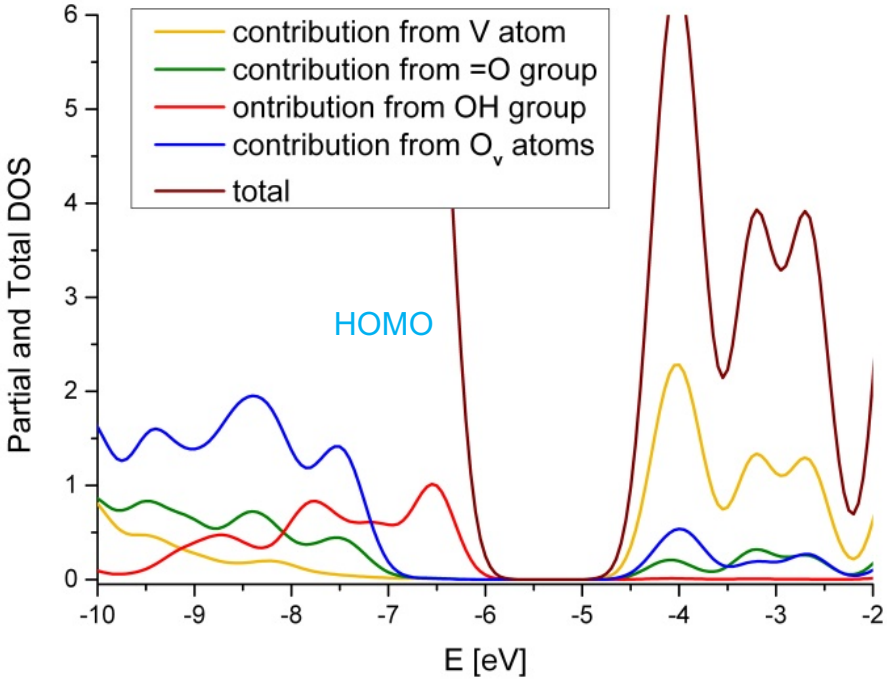

Figure S31. DOS plot for the system in which V-O center is in T6 position

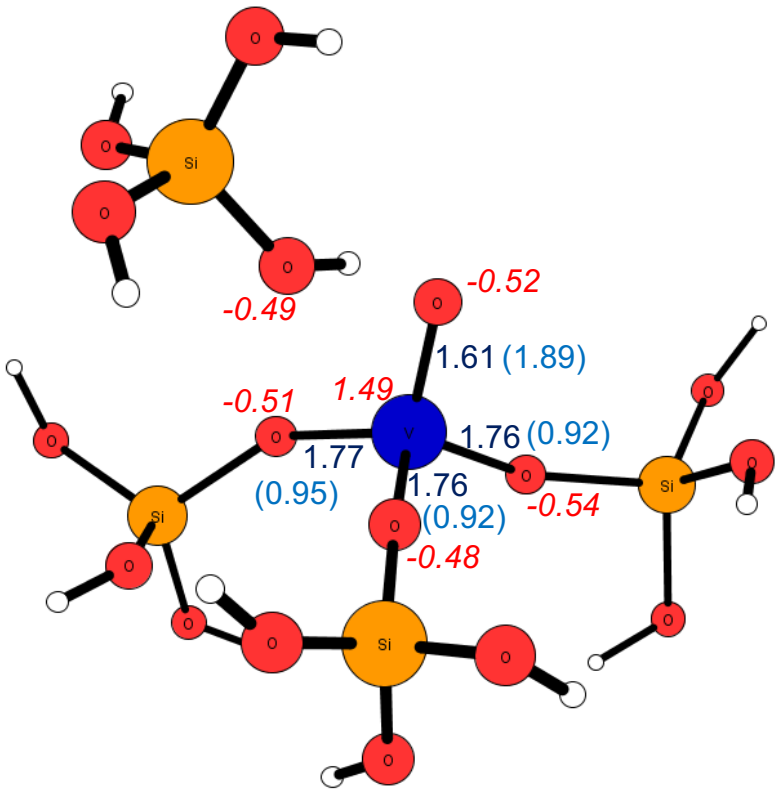

Figure S32. Computed parameters of V-O center in T7 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges **).**

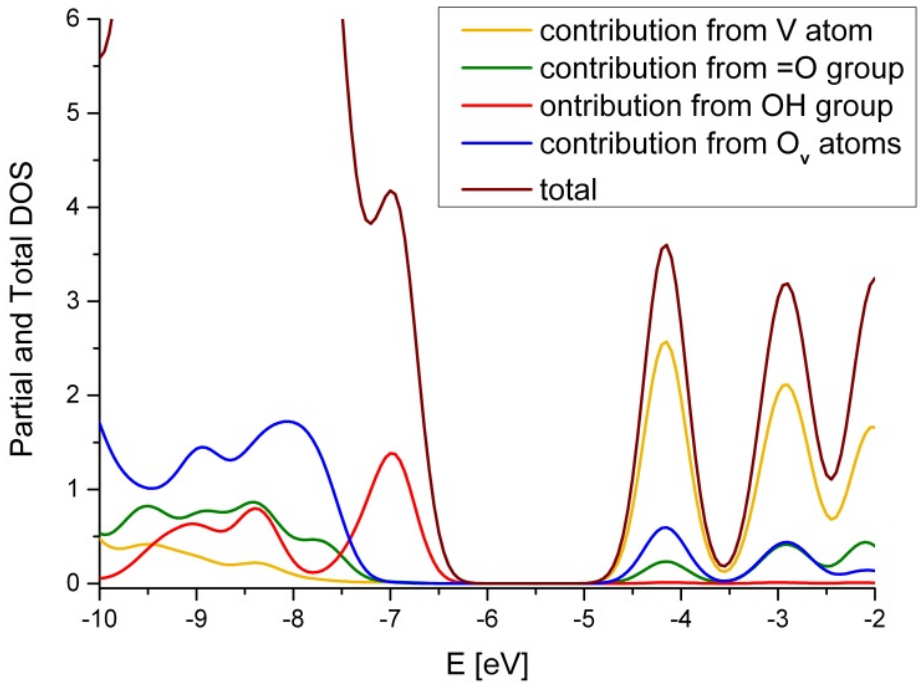

Figure S33. DOS plot for the system in which V-O center is in T7 position

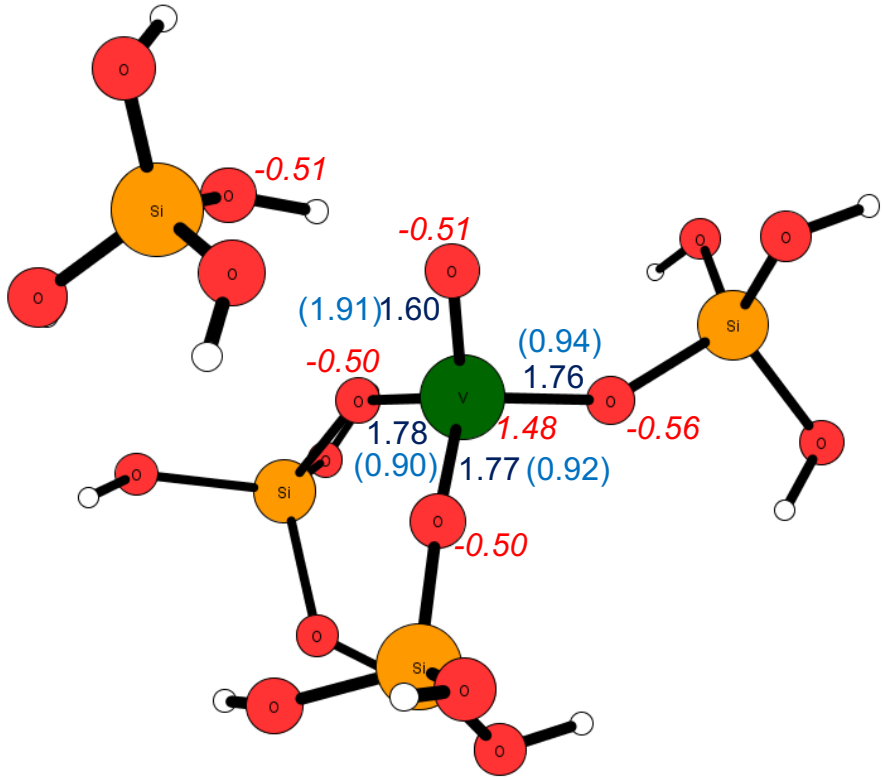

Figure S34. Computed parameters of V-O center in T8 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

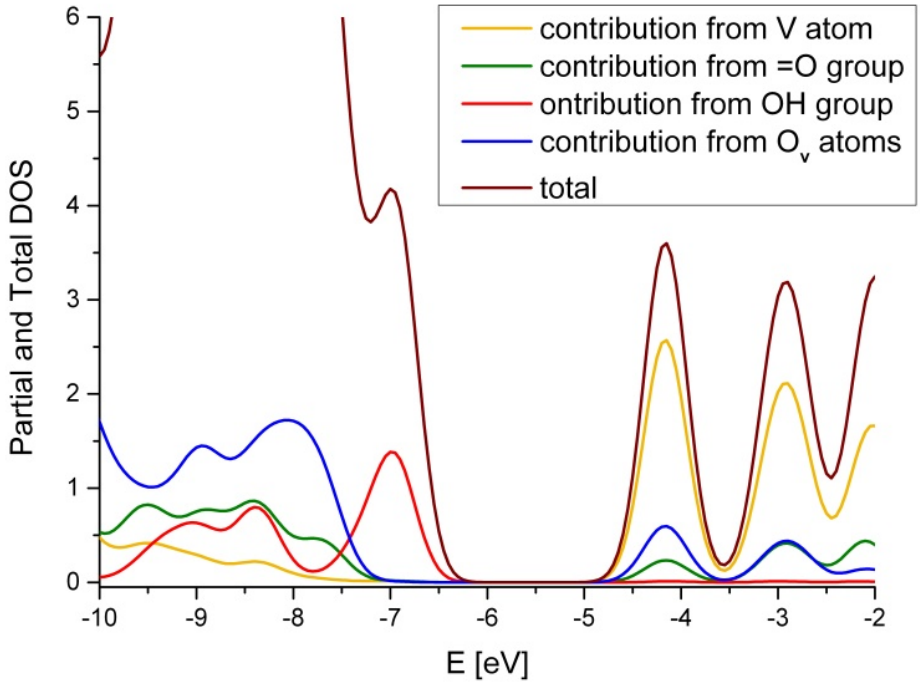

Figure S35. DOS plot for the system in which V-O center is in T8 position

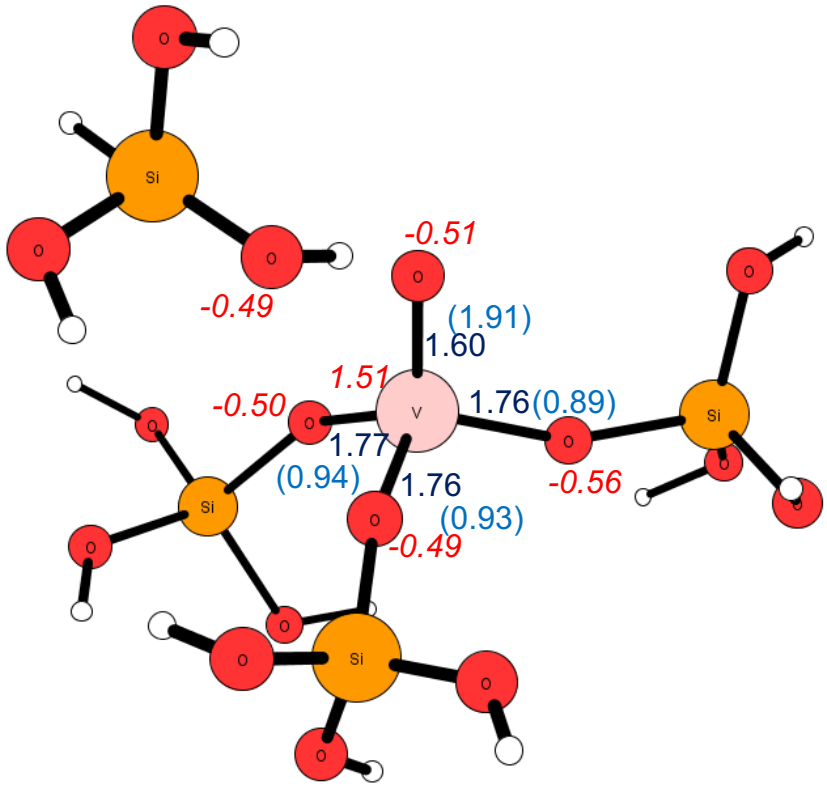

Figure S36. Computed parameters of V-O center in T9 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

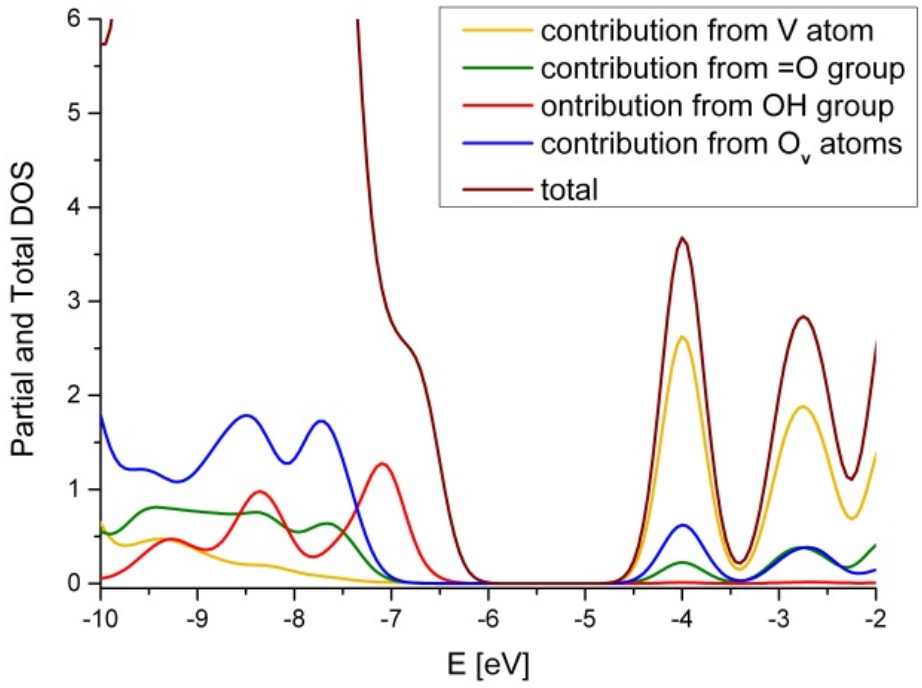

Figure S37. DOS plot for the system in which V-O center is in T9 position

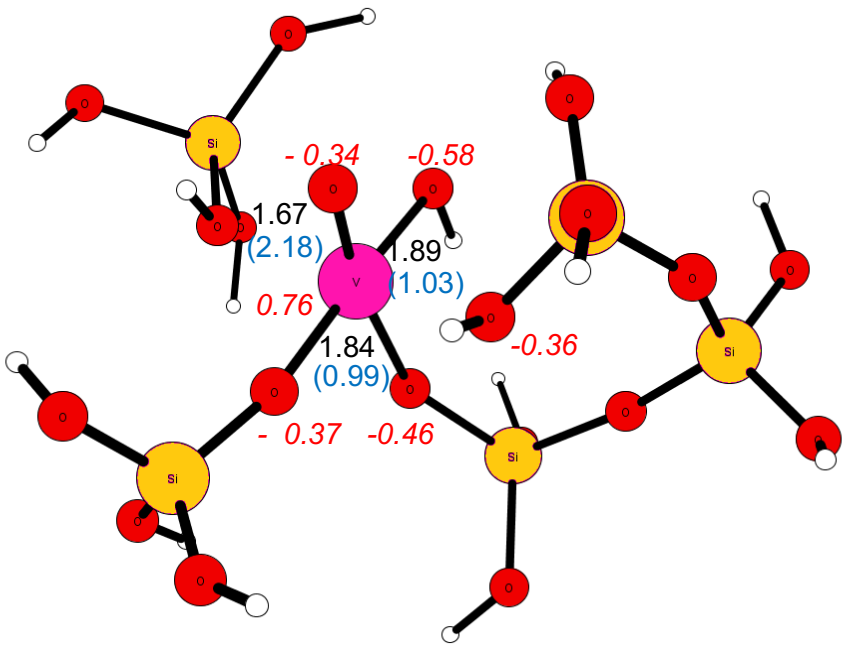

Figure S38. Computed parameters of V-O(OH) center in T1 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

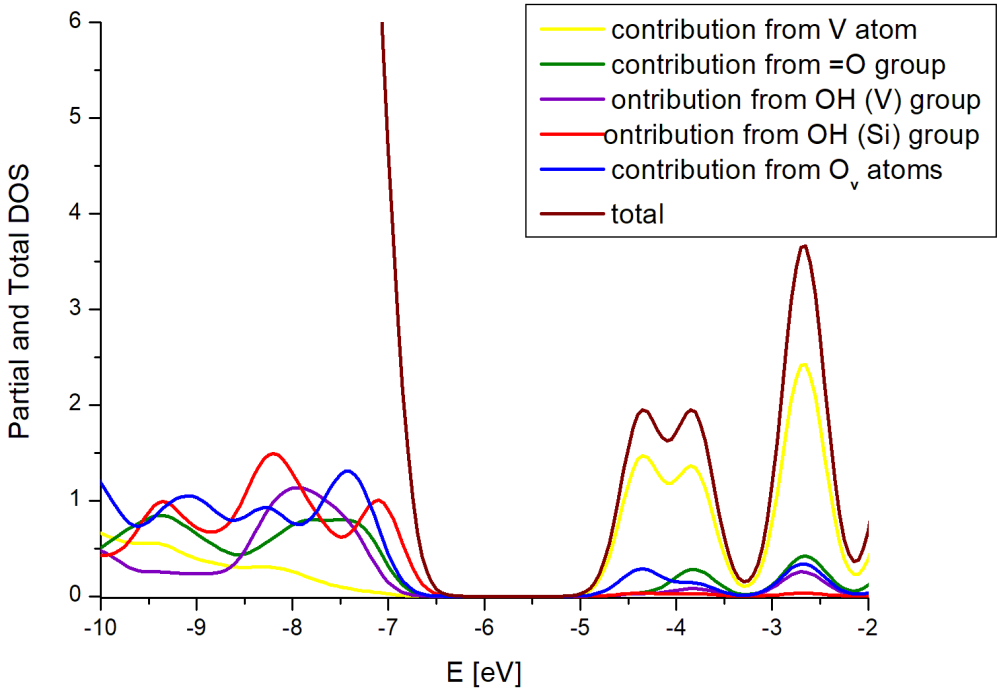

Figure S39. DOS plot for the system in which V-O(OH) center is in T1 position.

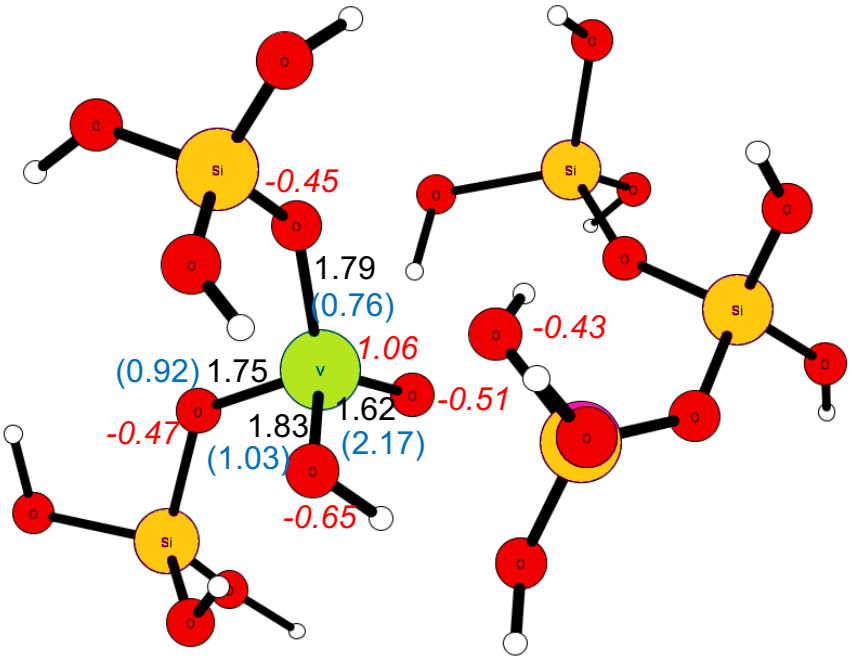

Figure S40. Computed parameters of V-(O)OH center in T2 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

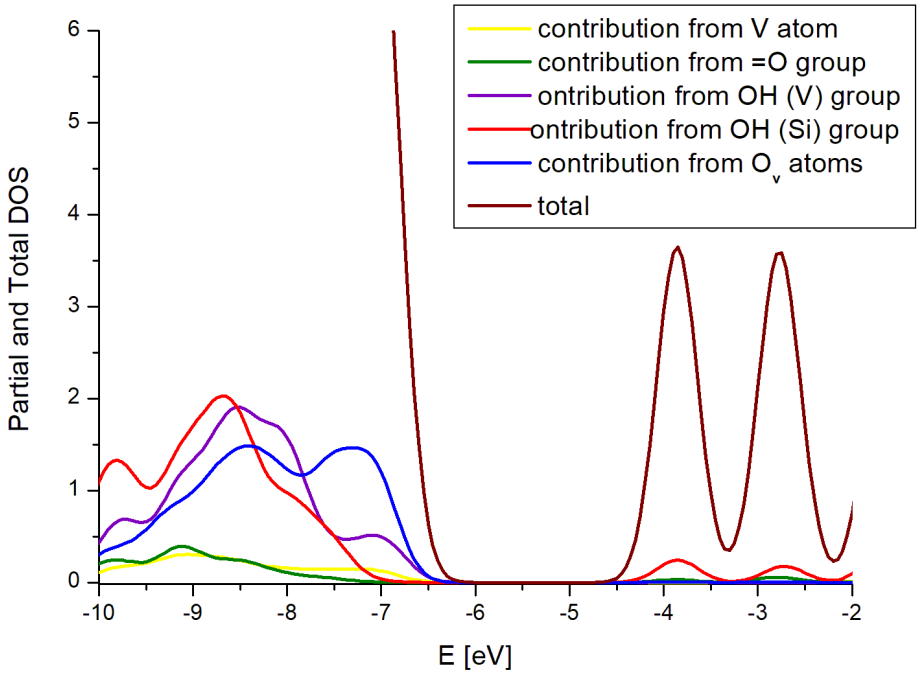

Figure S41. DOS plot for the system in which V-O(OH) center is in T2 position.

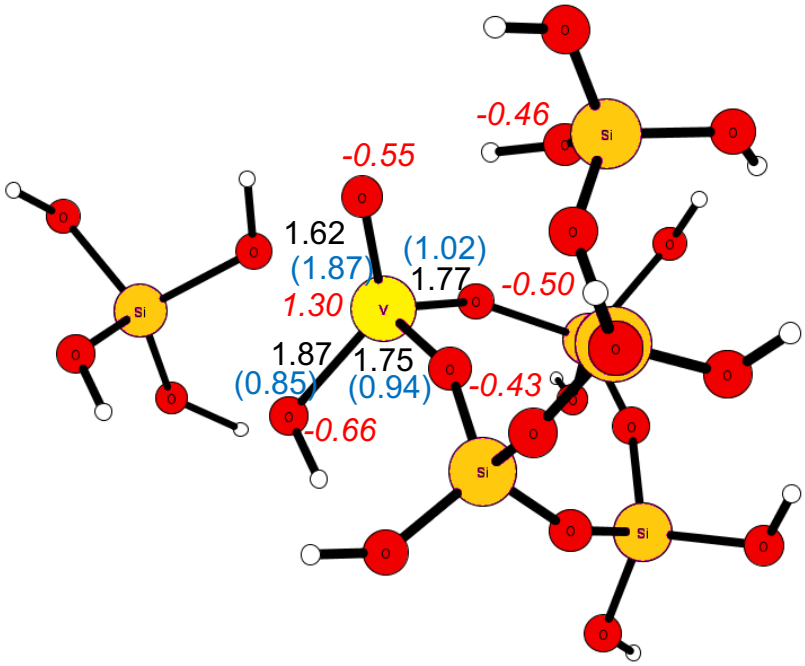

Figure S42. Computed parameters of V-O(OH) center in T3 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

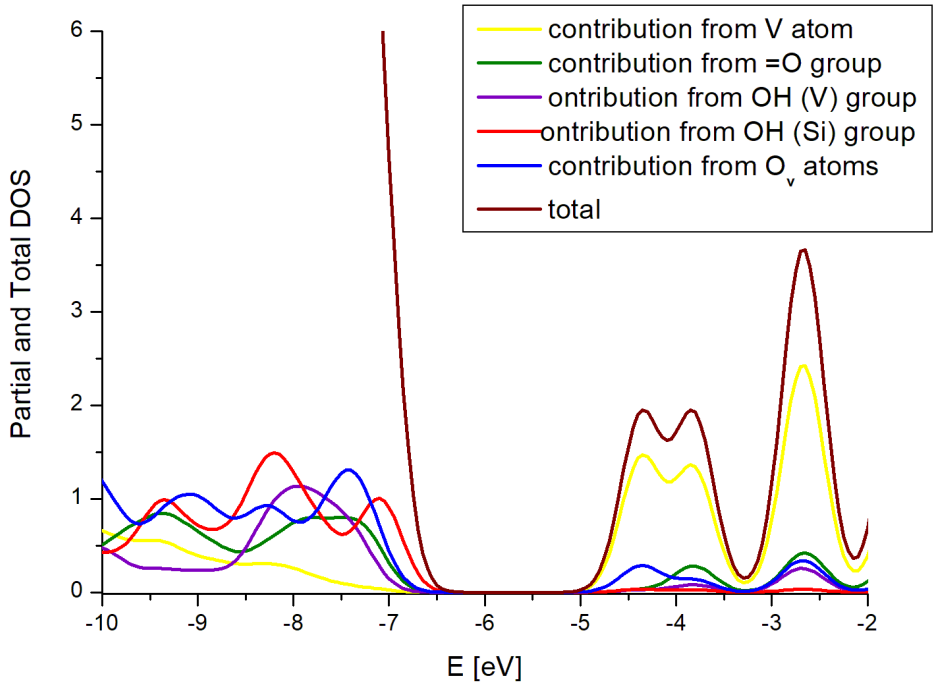

Figure S43. DOS plot for the system in which V-(O)OH center is in T3 position.

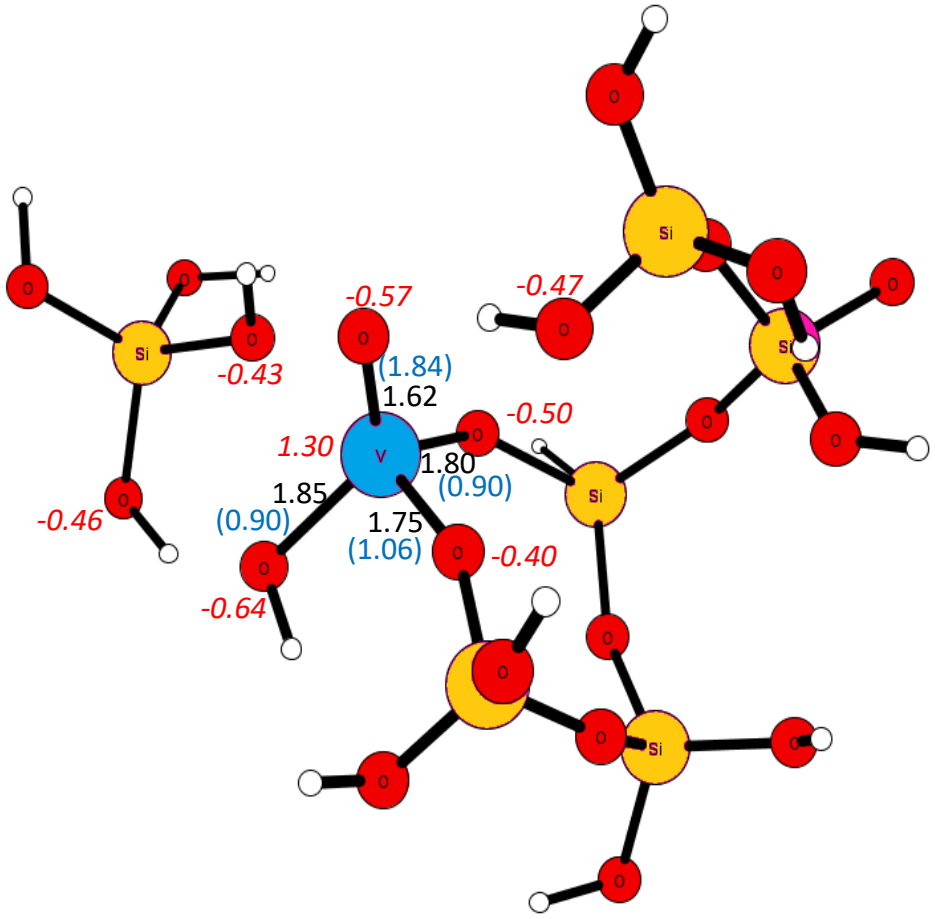

Figure S44. Computed parameters of V-(O)OH center in T4 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges **).**

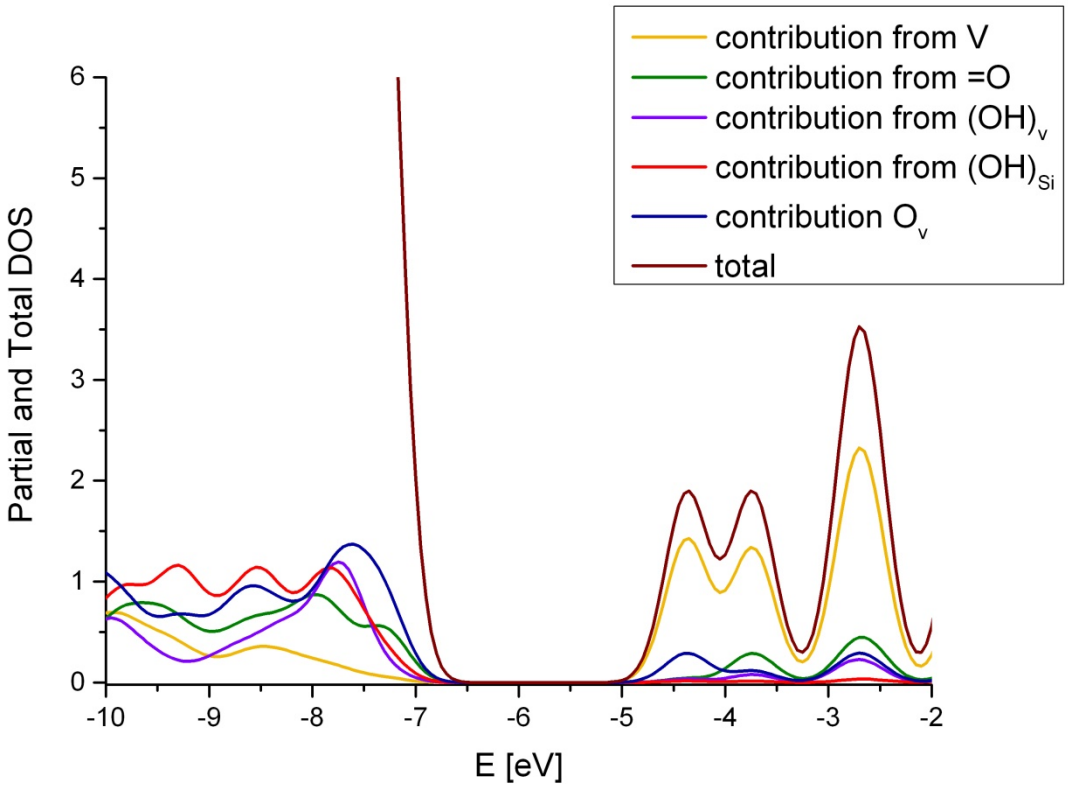

Figure S45. DOS plot for the system in which V-(O)OH center is in T4 position.

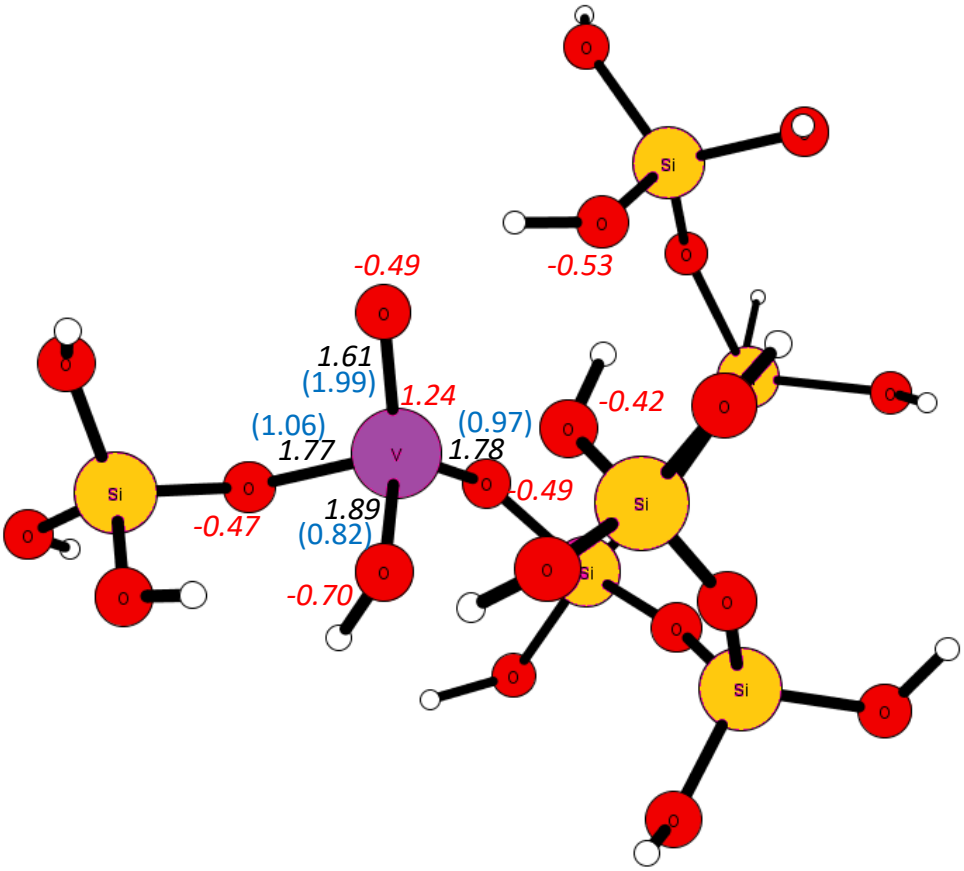

Figure S46. Computed parameters of V-O(OH) center in T5 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

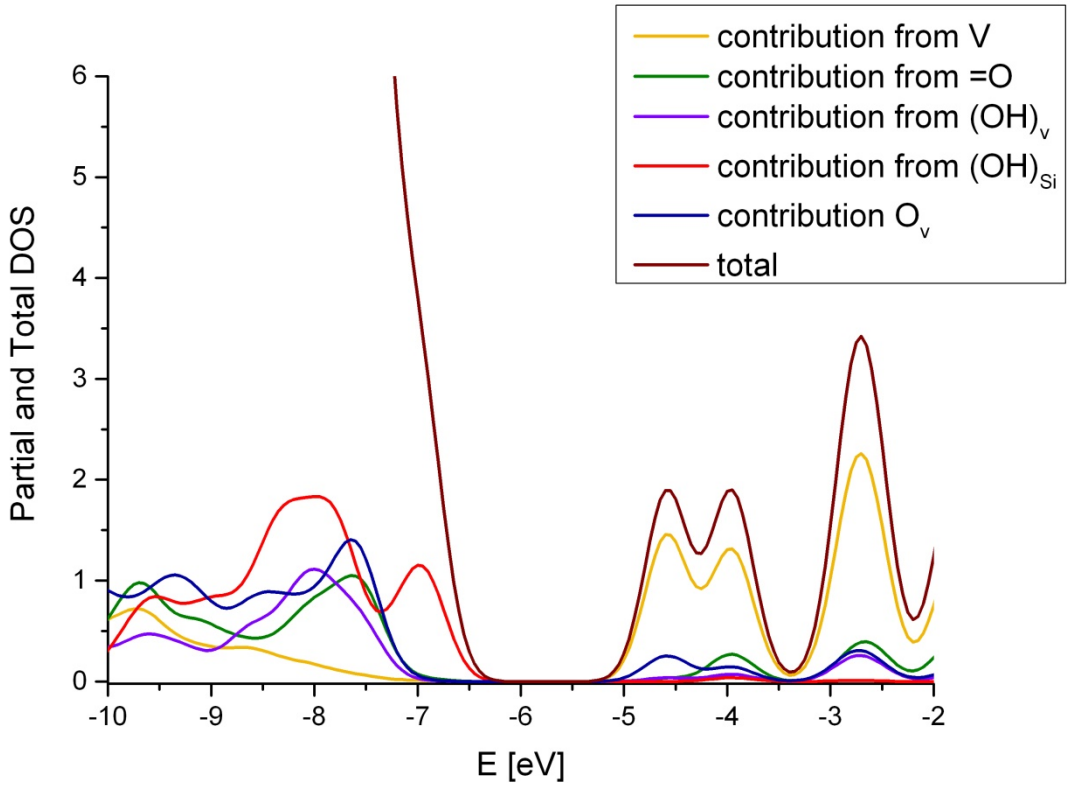

Figure S47. DOS plot for the system in which V-O(OH) center is in T5 position.

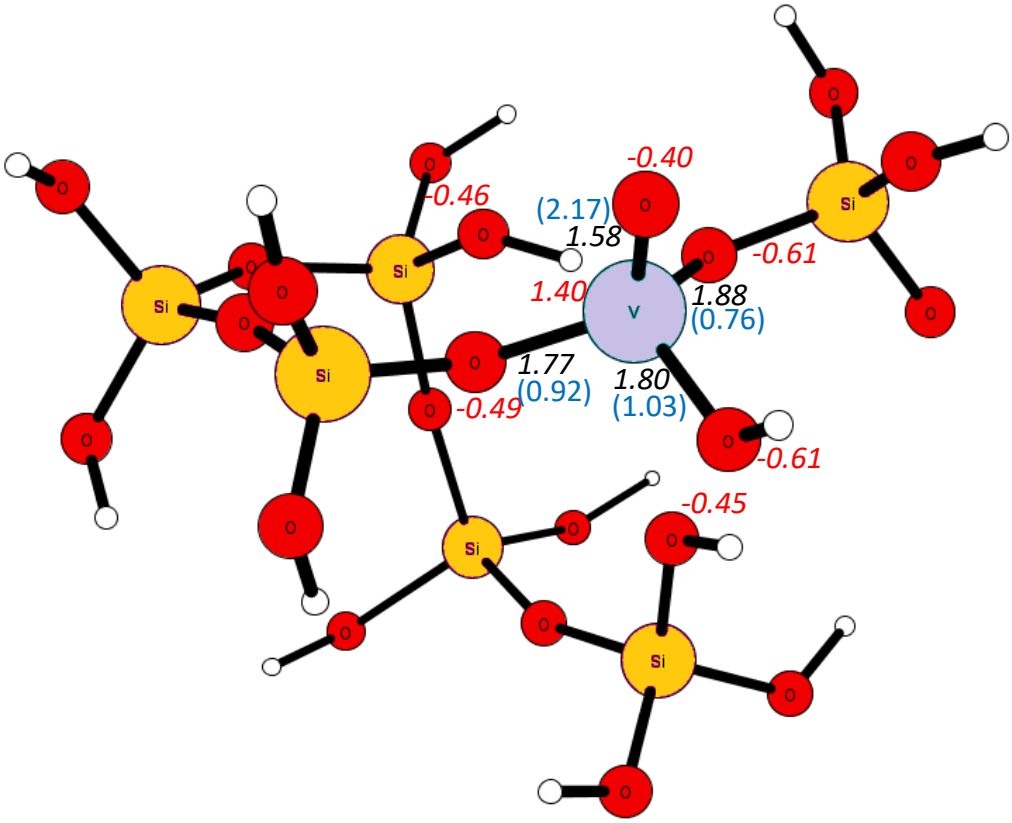

Figure S48. Computed parameters of V-(O)OH center in T6 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

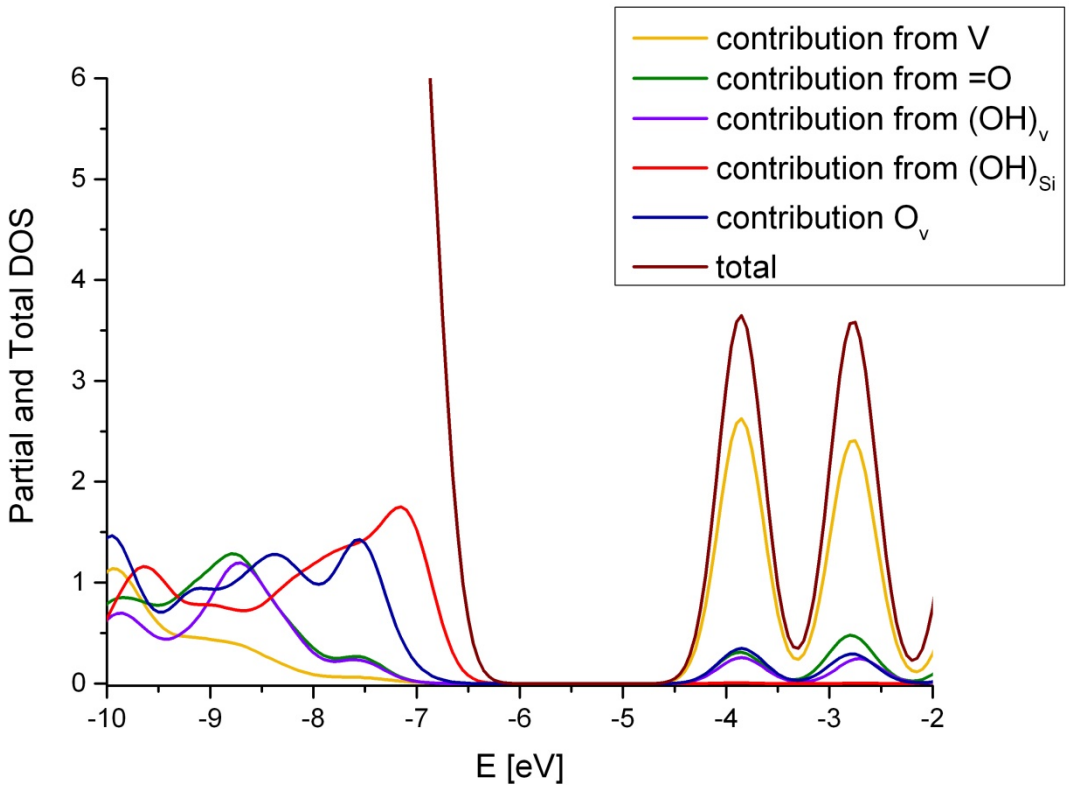

Figure S49. DOS plot for the system in which V-O(OH) center is in T6 position.

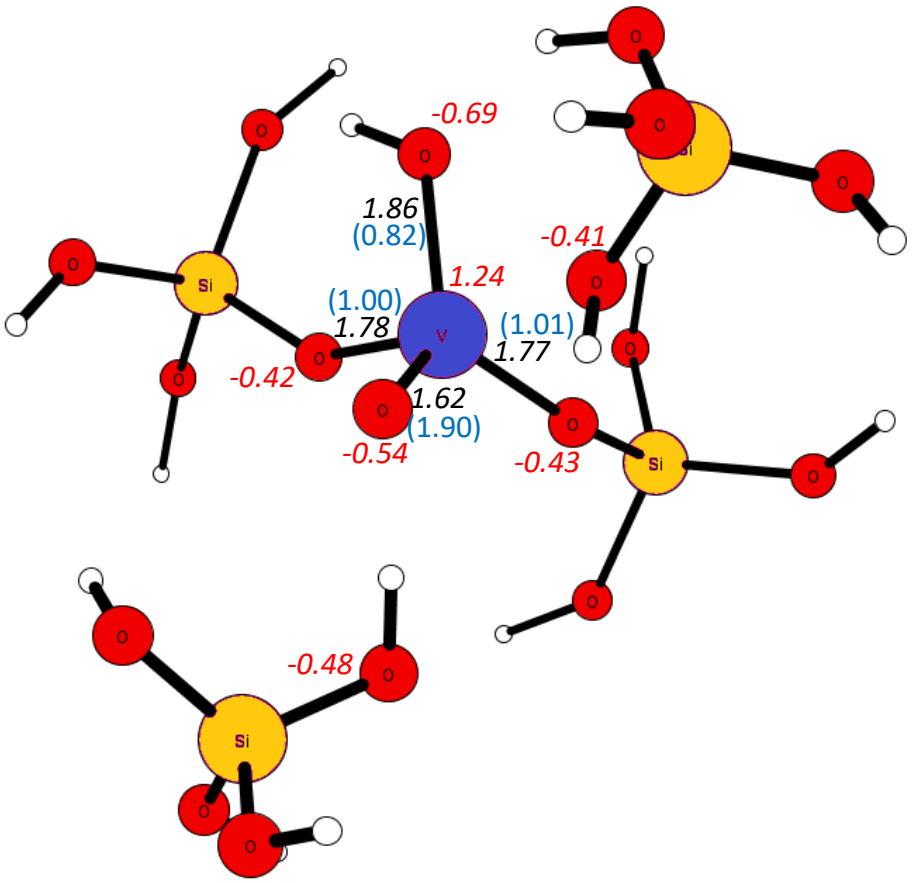

Figure S50. Computed parameters of V-O(OH) center in T7 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

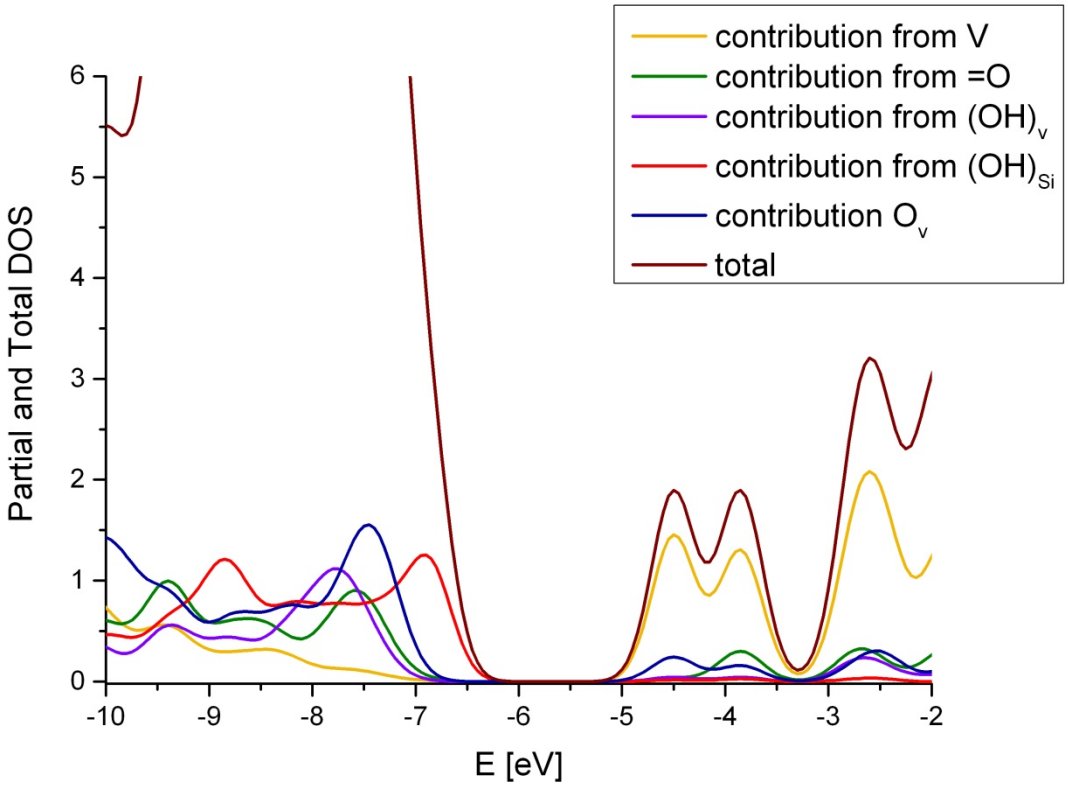

Figure S51. DOS plot for the system in which V-O(OH) center is in T7 position.

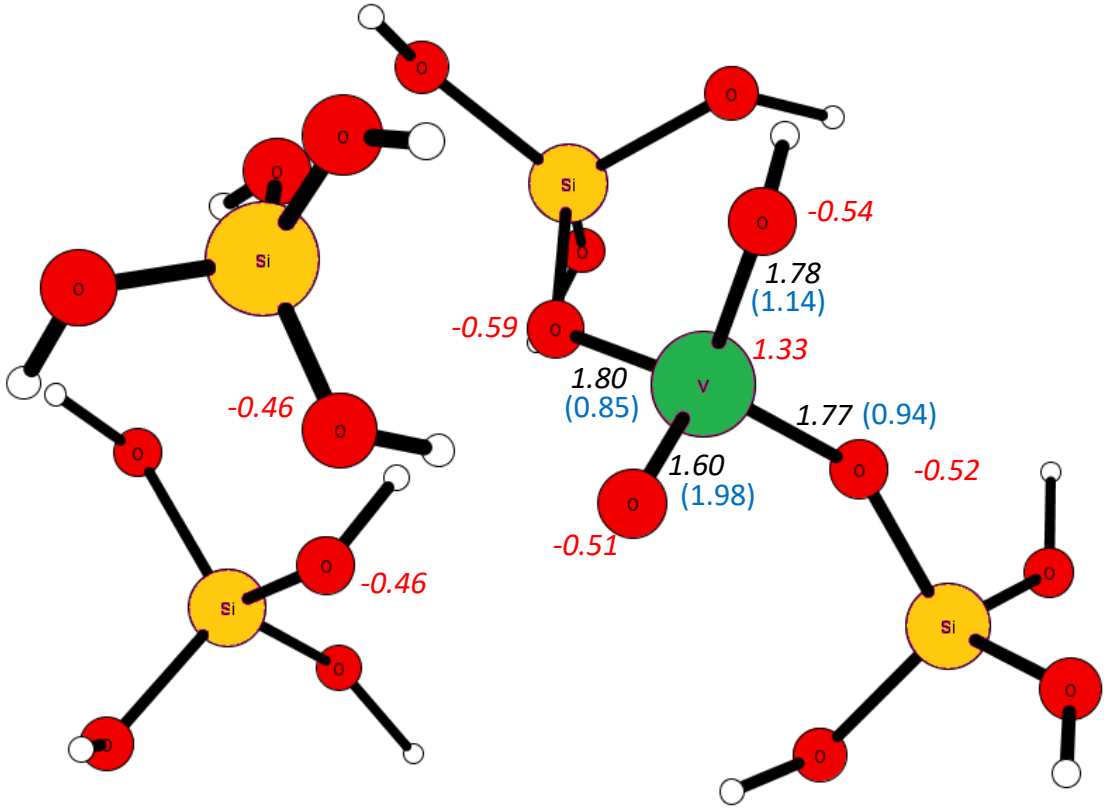

Figure S52. Computed parameters of V-O(OH) center in T8 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

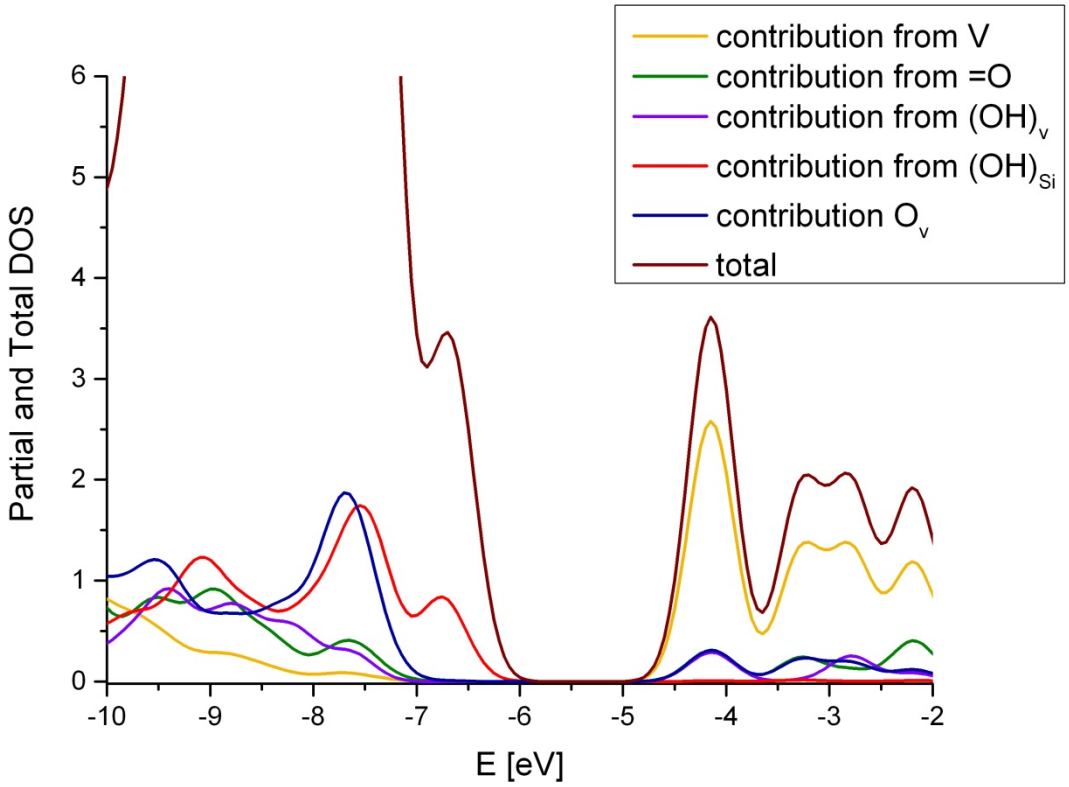

Figure S53. DOS plot for the system in which V-O(OH) center is in T8 position.

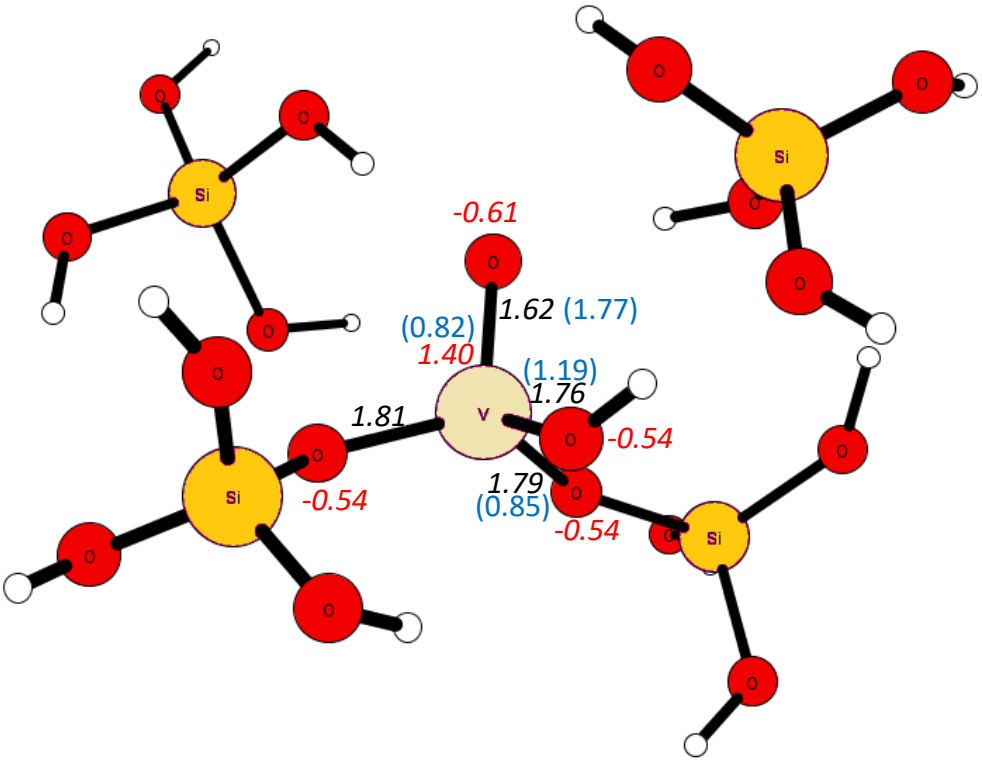

Figure S54. Computed parameters of V-O(OH) center in T9 position (black - bond lengths in Å; blue, in parentheses – bond order indices; red – Mulliken charges).

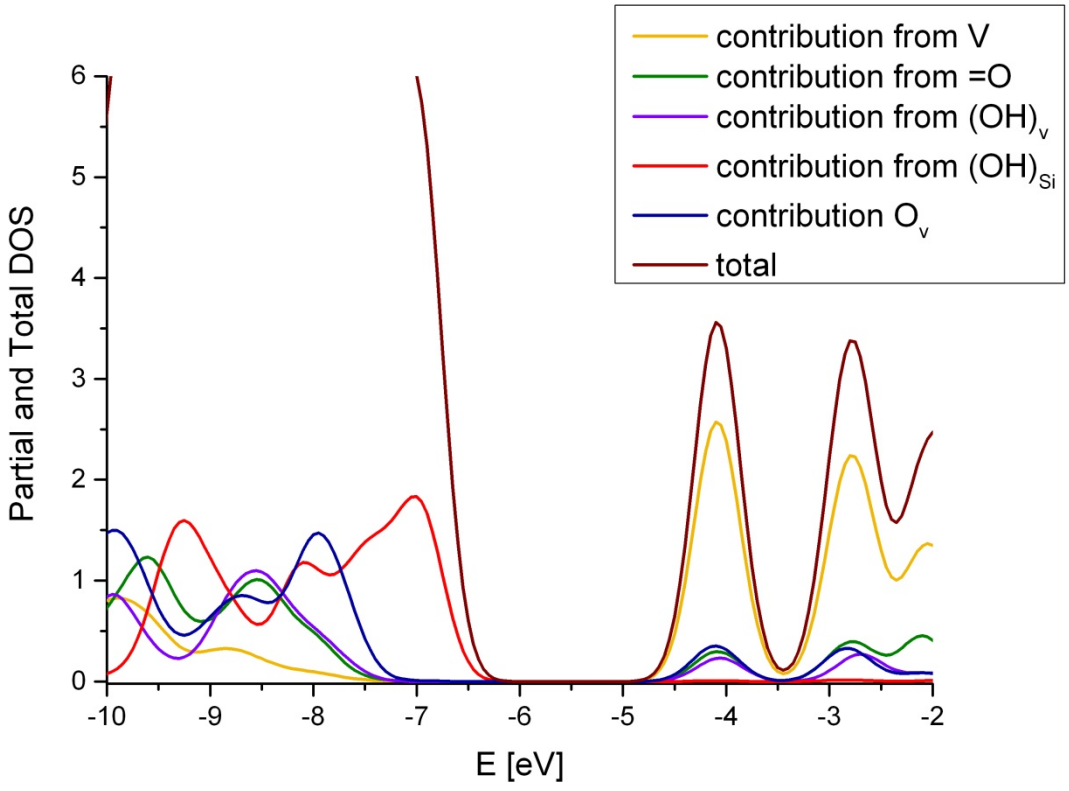

Figure S55. DOS plot for the system in which V-O(OH) center is in T9 position.

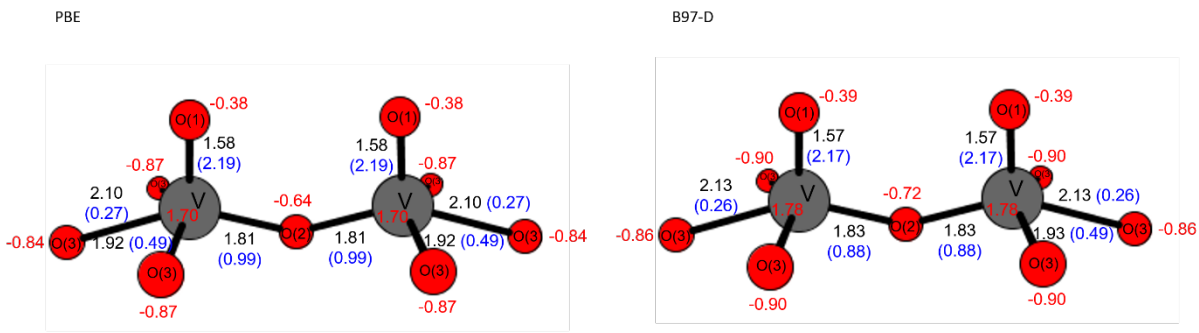

Figure S56. Comparison of the computed parameters (Mulliken charges at selected atoms, bond distances [Å] and Mayer bond order indices) with PBE and B97-D functionals: $V_{20}O_{62}H_{24}$ cluster.

Table S1. Comparison of the selected parameters for V-OH (T3 site) as a function of the cluster size.

V atom number		PBE functional	B97-D functional	Relative change
		V-V distance [Å]		
33	85	4,64	4,99	7,5%
34	86	4,64	4,99	7,5%
35	87	4,64	4,67	0,6%
36	88	4,64	4,67	0,6%
37	89	4,64	4,67	0,6%
38	90	4,64	4,67	0,6%
39	91	4,64	4,77	2,8%
40	92	4,64	4,77	2,8%
41	93	4,64	4,77	2,8%
42	94	4,64	4,77	2,8%

Table S2: Distances [Å] between vanadium atoms from the first and the second layer of the $V_{20}O_{62}H_{24}$ cluster computed with B97-D functional.

T3 model	**dV-OH [Å]**	**BO**	**qOoh**	**qOH**	**qV**
small	1.81	1.13	-0.49	-0.14	1.40
medium	1.82	1.12	-0.48	-0.16	1.37
big	1.84	1.13	-0.52	-0.18	0.96

T3 model	**dV=O [Å]**	**BO**	**qO**	**qV**
small	1.60	1.83	-0.49	1.43

medium	1.60	1.93	-0.50	1.50
big	1.62	1.91	-0.52	0.95