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Supporting information for:

Structural and Decomposition Analysis of TKX-50 with Vacancy Defects: Insights from DFT and AIMD Simulations

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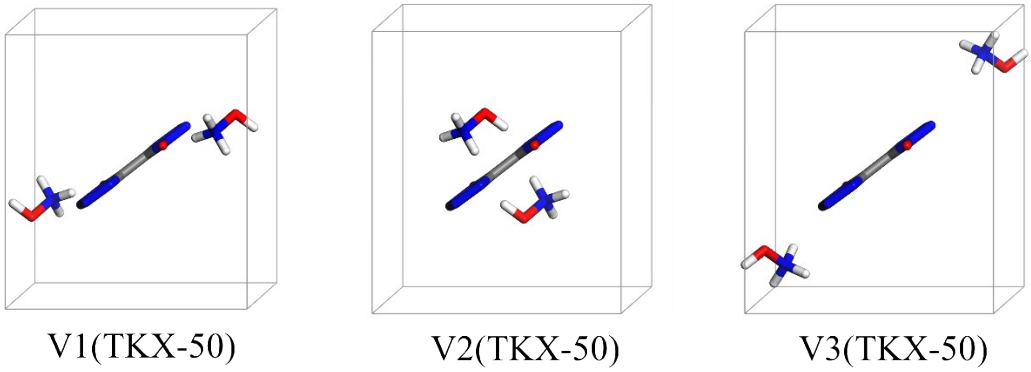

Fig.S1 The isolated TKX-50 models in V1-V3 system

As shown in Figure S1, the TKX-50 in the model are the anions and cations deleted when creating the defective system.

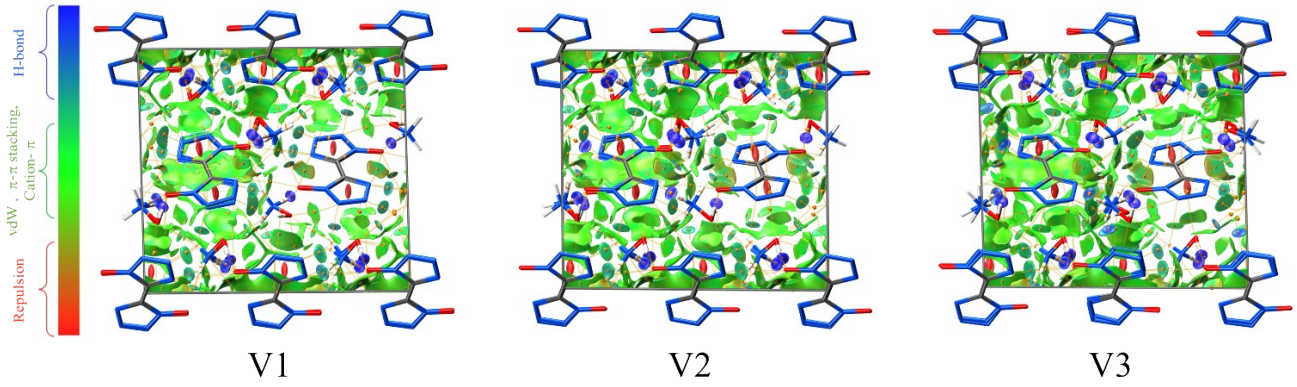

Fig.S2 Colored isosurfaces of the noncovalent interactions of V1-V3 by NCI analysis

Table S1 The potential energy density V(r), hydrogen bond energy E_{HB} (kcal mol^{-1}), the electron density ρ(r), Laplacian value $\nabla^2\rho$(r) and the energy density H(r) at the bond critical points (BCPs) for the noncovalent interactions of V0-V3

		Connected atoms	Interaction type	ρ(r) [a.u.]	V(r) [a.u.]	E_{HB} [kcal mol^{-1}]	H(r) [a.u.]	$\nabla^2\rho$(r) [a.u.]
(a) and (e)	1	O2---H5C	H-bond	0.012	-0.0078	-2.46	0.003	0.051
	2	O2---N4	Cation-π	0.005	-0.0025	\	0.001	0.020
	3	H5C---N2	H-bond	0.013	-0.0082	-2.57	0.002	0.051
	4	H5C---O2	H-bond	0.012	-0.0078	-2.45	0.003	0.051
	5	H5C---N3	H-bond	0.013	-0.0083	-2.60	0.002	0.051
	6	H5A---N4	H-bond	0.020	-0.0132	-4.13	0.001	0.063
	7	H5A---O1	H-bond	0.014	-0.0091	-2.87	0.002	0.055
	8	N5---N4	vdW	0.005	-0.0029	\	0.001	0.022
	9	H5B---O1	H-bond	0.045	-0.0383	-12.03	-0.005	0.113
	10	H2---O1	H-bond	0.063	-0.0602	-18.90	-0.015	0.122
(b)	1	O2---H5C	H-bond	0.010	-0.0057	-1.79	0.002	0.042
	2	O2---C1	Cation-π	0.005	-0.0027	\	0.001	0.022
	3	N5---N2	vdW	0.008	-0.0052	\	0.002	0.036
	4	H5C---O2	H-bond	0.012	-0.0074	-2.33	0.002	0.050
	5	H5C---N3	H-bond	0.016	-0.0103	-3.22	0.002	0.057
	8	H5A---N4	H-bond	0.009	-0.0046	-1.44	0.002	0.032
	9	H5B---O1	H-bond	0.066	-0.0635	-19.91	-0.017	0.121
	10	H2---O1	H-bond	0.070	-0.0698	-21.90	-0.020	0.121
(c)	1	O2---H5C	H-bond	0.013	-0.0086	-2.70	0.002	0.054
	2	O2---C1	Cation-π	0.006	-0.0030	\	0.001	0.024
	3	N5---N2	vdW	0.007	-0.0043	\	0.002	0.031
	4	H5C---O2	H-bond	0.010	-0.0056	-1.76	0.002	0.041
	5	H5C---N3	H-bond	0.014	-0.0082	-2.58	0.002	0.049
	8	H5A---N4	H-bond	0.028	-0.0188	-5.91	0.000	0.076
	9	H5B---O1	H-bond	0.045	-0.0385	-12.08	-0.005	0.114
	10	H2---O1	H-bond	0.084	-0.0907	-28.45	-0.031	0.113
(d)	1	O2---H5C	H-bond	0.011	-0.0067	-2.11	0.002	0.047
	2	O2---N4	Cation-π	0.007	-0.0039	\	0.002	0.029
	3	N5---N2	vdW	0.012	-0.0081	\	0.002	0.052
	4	H5C---O2	H-bond	0.022	-0.0158	-4.96	0.002	0.076
	5	N5---N3	vdW	0.012	-0.0074	\	0.002	0.048
	8	H5A---N4	H-bond	0.008	-0.0045	-1.43	0.002	0.032
	9	H5B---O1	H-bond	0.040	-0.0334	-10.48	-0.004	0.105
	10	H2---O1	H-bond	0.070	-0.0703	-22.07	-0.020	0.121
(f)	1	O2---H5C	H-bond	0.006	-0.003	-0.99	0.002	0.027

	2	O2---N4	Cation-π	0.004	-0.002	\	0.001	0.017
	3	H5C---N2	H-bond	0.016	-0.010	-3.21	0.002	0.057
	4	H5C---O2	H-bond	0.012	-0.008	-2.49	0.002	0.052
	5	N5---N3	vdW	0.015	-0.010	\	0.003	0.059
	6	H5A---N4	H-bond	0.017	-0.011	-3.43	0.002	0.057
	7	H5A---O1	H-bond	0.014	-0.009	-2.79	0.002	0.053
	9	H5B---O1	H-bond	0.075	-0.076	-23.73	-0.024	0.111
	11	O2---N2	vdW	0.004	-0.002	\	0.001	0.018
	12	H2---N2	H-bond	0.005	-0.002	-0.77	0.001	0.020
(g)	1	O2---H5C	H-bond	0.016	-0.0106	-3.31	0.002	0.061
	2	O2---N4	Cation-π	0.006	-0.0034	\	0.002	0.026
	3	H5C---N2	H-bond	0.017	-0.0108	-3.39	0.002	0.057
	4	N5---O2	vdW	0.008	-0.0047	\	0.002	0.036
	5	H5C---N3	H-bond	0.013	-0.0077	-2.41	0.002	0.047
	6	H5A---N4	H-bond	0.047	-0.0359	-11.25	-0.006	0.097
	7	N5---O1	vdW	0.010	-0.0063	\	0.002	0.045
	8	N5---N4	H-bond	0.020	-0.0130	-4.08	0.001	0.063
	10	H2---O1	H-bond	0.083	-0.0891	-27.97	-0.031	0.108
(h)	1	O2---H5C	H-bond	0.004	-0.0021	-0.67	0.001	0.020
	3	H5C---N2	H-bond	0.023	-0.0163	-5.11	0.001	0.077
	4	H5C---O2	H-bond	0.013	-0.0088	-2.76	0.003	0.055
	5	N5---N3	vdW	0.013	-0.0083	\	0.002	0.053
	6	H5A---N4	H-bond	0.013	-0.0078	-2.45	0.002	0.047
	7	H5A---O1	H-bond	0.028	-0.0211	-6.63	0.000	0.086
	9	H5B---O1	H-bond	0.051	-0.0463	-14.53	-0.008	0.122
	11	O2---N2	vdW	0.003	-0.0015	\	0.001	0.014
	12	H2---N2	H-bond	0.007	-0.0036	-1.12	0.002	0.027
	13	H2---N4	H-bond	0.009	-0.0049	-1.54	0.002	0.034

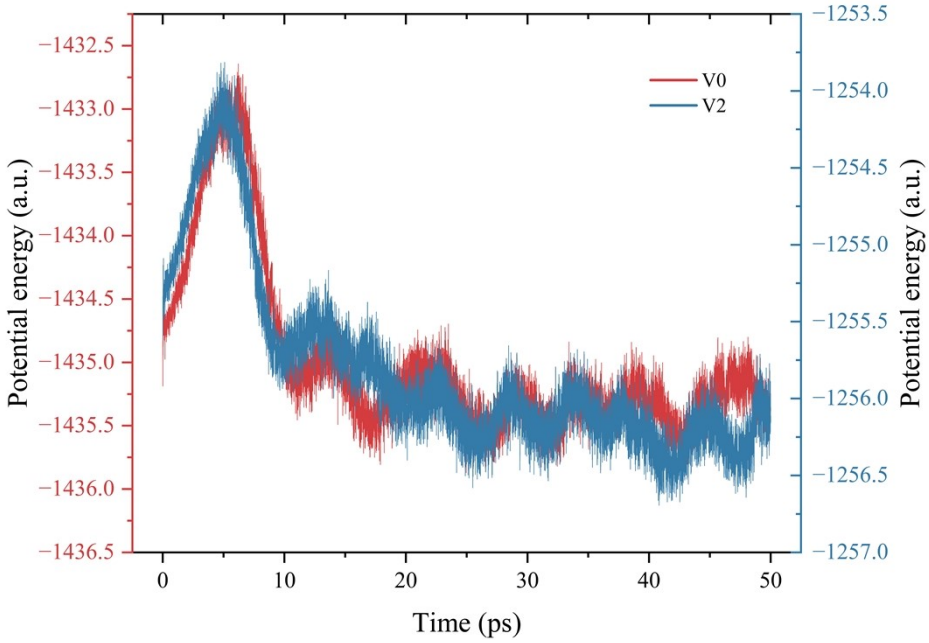

Fig.S3 Potential energy evolution curves of V0 and V2 systems

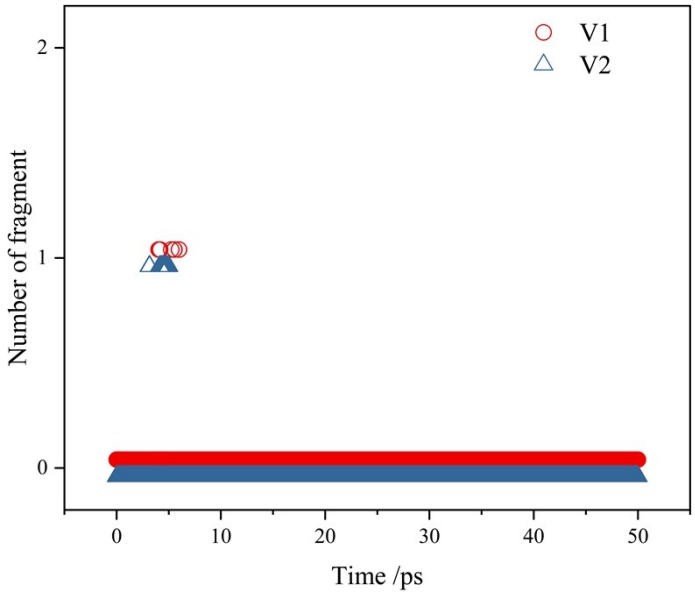

Fig.S4 The evolution of ABTOX