Supporting Information

Adsorption and sensing properties of Methyl Acetate on VTe2 Doped Systems (Ti, Sc, Ru, Y) from First-Principles

Guan-Nan Wang [a,b], *Hong Zhang* [a,b,*]

[a] College of Physics, Sichuan University, Chengdu 610065, China

[b] Key Laboratory of High Energy Density Physics and Technology (Ministry of Education), Sichuan University, Chengdu 610065, China

[*] Corresponding author: Hong Zhang.

Email address: hongzhang@scu.edu.cn (Hong Zhang).

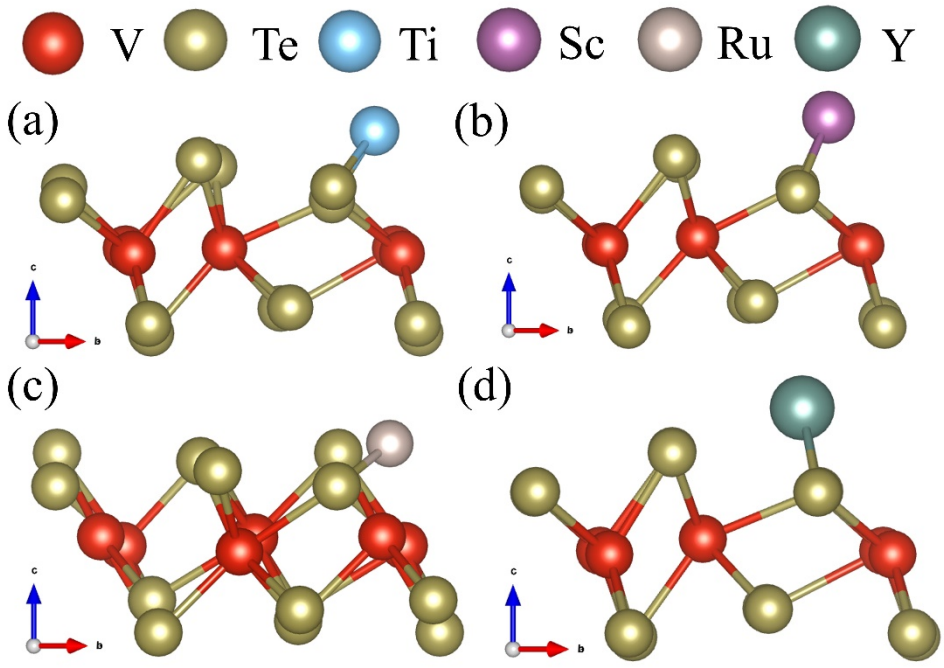

Figure S1. AIMD simulations for (a) VTe2+Ti, (b) VTe2+Sc, (c) VTe2+Ru, and (d) VTe2+Y.

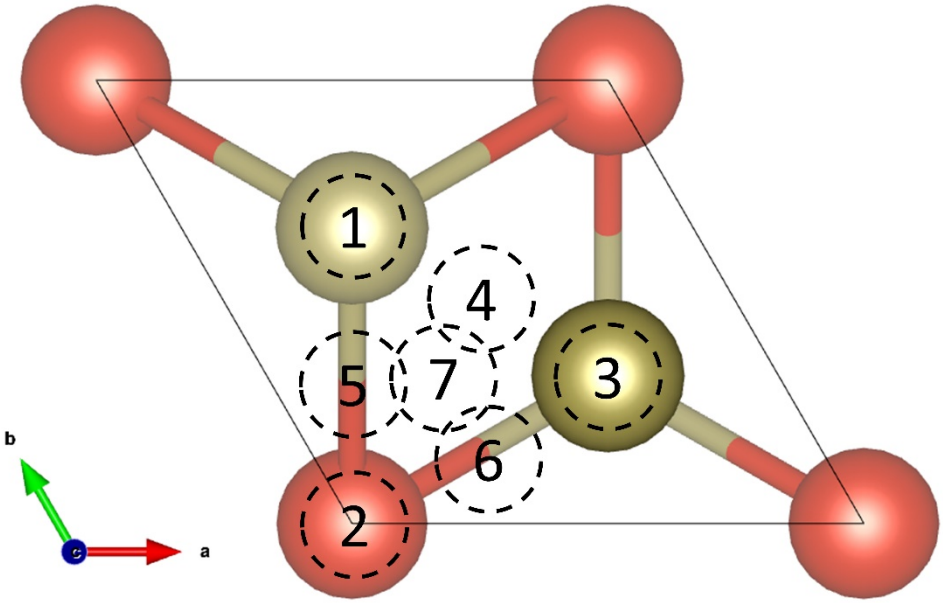

Figure S2. Adsorption sites for methyl acetate on the surface of VTe_2, 1, 2, and 3 correspond to the top, hcp, and fcc sites.

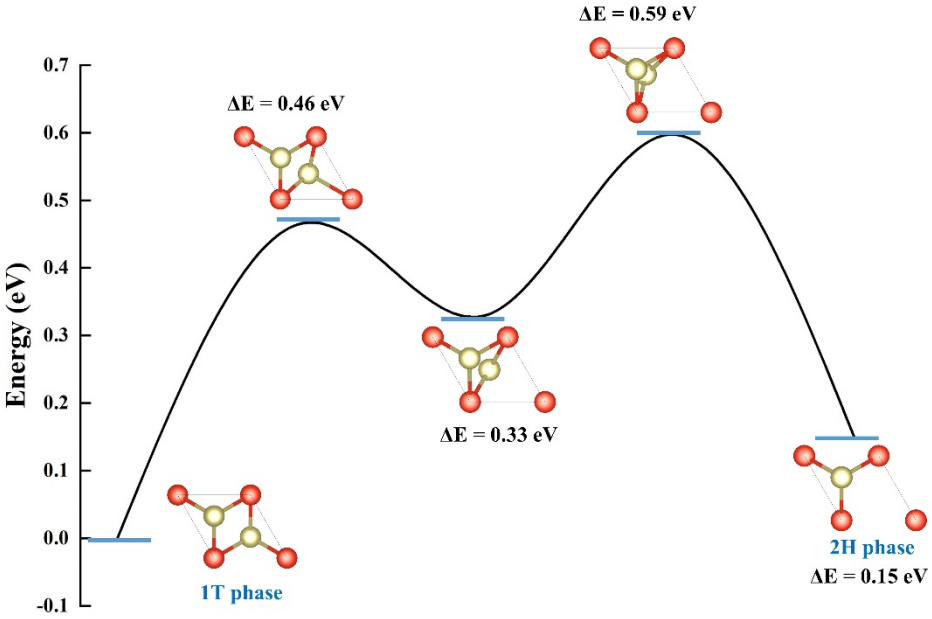

Figure S3. Phase transition curves of 1T and 2H phases within a single cell of VTe_2, and the energy obtained from DFT calculations.

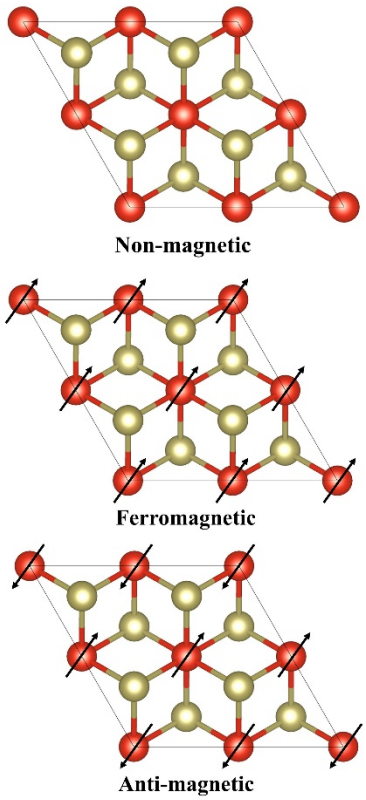

Figure S4 The three considered magnetic configurations of VTe_2 are non-magnetic, ferromagnetic, and antiferromagnetic.

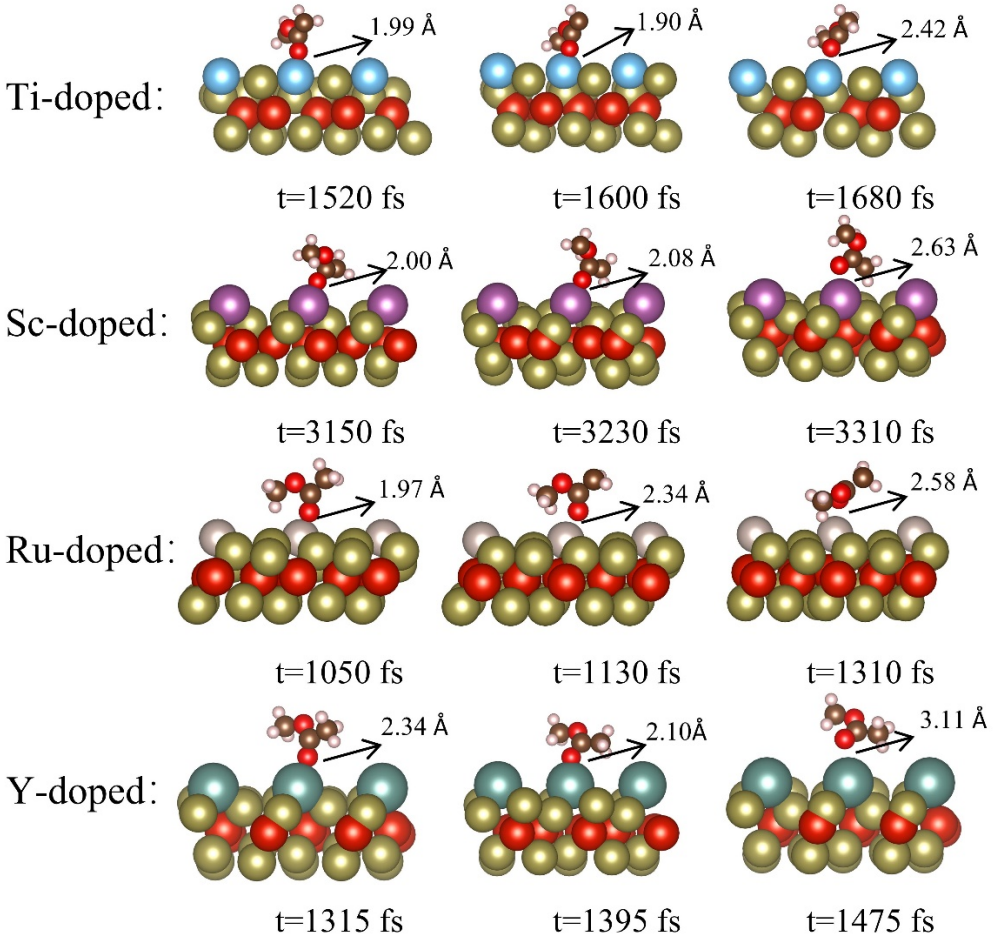

Figure S5. The partial trajectories and distances of molecular desorption at 800K.

Table S1. The adsorption energies of methyl acetate molecules at seven different sites.

site	Potential energy (eV)	Adsorption energy(eV)
1 (top)	-116.00	-0.18
2 (hcp)	-116.02	-0.20
3 (fcc)	-116.16	-0.34
4	-115.61	+0.21
5	-115.71	+0.11
6	-116.16	-0.34
7	-115.87	-0.05

Table S2. The adsorption energies of several candidate metal atoms and the adsorption energies of methyl acetate gas on their doped surfaces.

Metal atom	Adsorption energy for metal atoms (eV)	Adsorption energy for molecule (eV)
Fe	-3.56	-0.09
Al	-2.98	-0.06
Cu	-1.75	-1.75
Zn	+0.09	——
Mn	+1.16	——
Mg	-1.68	-1.68
Mo	-1.01	-3.44
Ni	-4.38	0.38

Table S3. Spin up, spin down, and total band gap upon doping.

Structure	Spin Up (meV)	Spin Down (meV)	Total Band Gap (meV)
VTe2+Ti	9.7	15.3	9.7
VTe2+Sc	9.1	18.8	9.1
VTe2+Ru	19.0	9.5	5.0
VTe2+Y	13.4	31.9	13.4

Table S4. Coordinates for the Ti-doped system.

	X	Y	Z
V	-0.0413493327147601	0.0200397159537981	0.1005526545751598
V	0.4649609914016448	0.0516209258480980	0.0961226299367035
V	0.0147329652717953	0.4931940444276510	0.1014881098605952
V	0.4629667034563535	0.4845638543781143	0.0965739889553835
Te	0.3085200620226728	0.3458085996592411	0.9906555664355446
Te	0.1572631010020561	0.1548779963889998	0.2062375496026223
Te	0.8103521821528216	0.3511461091614472	0.0058926859229011
Te	0.6449090853449800	0.1773713962442842	0.2032399788097209
Te	0.3074320971601283	0.8462446904974306	0.0091134778521925
Te	0.1564408545001195	0.6873653057754332	0.2071458941321989
Te	0.8103796979701151	0.8377802250413150	0.0053237554343153
Te	0.6275709548444988	0.6861257214004672	0.1845449604171530
Te	0.9525705526018799	0.5220913770571691	0.2649187760280349

Table S5. Coordinates for the Sc-doped system.

	X	Y	Z
V	-0.0451766074501604	0.0134358135222976	0.1004636425942522
V	0.4937553296066067	0.0393131137034203	0.0955991176958591
V	0.0063254144535790	0.5120962290323625	0.0974688403517291
V	0.4558925396000622	0.4905777848843141	0.1005329115076292
Te	0.3080466078264945	0.3441889186913086	0.9930240501480312
Te	0.1569906593703373	0.1565960109249143	0.1946390801214208
Te	0.8102933594304783	0.3496505714439382	0.0089975695224231
Te	0.6434163010858376	0.1805499392362115	0.2042967099952168
Te	0.3086424718707251	0.8510723386385338	0.0107864887308197
Te	0.1487004844279736	0.6878271769492850	0.2090724401554652
Te	0.8116198656187131	0.8433266867054197	-0.0010050522514250
Te	0.6276953925037290	0.6857810161227620	0.1834852937860413
Ti	0.9505480966699278	0.5038143619786810	0.2744489356050633

Table S6. Coordinates for the Sc-doped system.

	X	Y	Z
V	-0.0451766074501604	0.0134358135222976	0.1004636425942522
V	0.4937553296066067	0.0393131137034203	0.0955991176958591
V	0.0063254144535790	0.5120962290323625	0.0974688403517291
V	0.4558925396000622	0.4905777848843141	0.1005329115076292
Te	0.3080466078264945	0.3441889186913086	0.9930240501480312
Te	0.1569906593703373	0.1565960109249143	0.1946390801214208
Te	0.8102933594304783	0.3496505714439382	0.0089975695224231
Te	0.6434163010858376	0.1805499392362115	0.2042967099952168
Te	0.3086424718707251	0.8510723386385338	0.0107864887308197
Te	0.1487004844279736	0.6878271769492850	0.2090724401554652

Te	0.8116198656187131	0.8433266867054197	-0.0010050522514250
Te	0.6276953925037290	0.6857810161227620	0.1834852937860413
Sc	0.9505480966699278	0.5038143619786810	0.2744489356050633

Table S7. Coordinates for the Ru-doped system.

	X	Y	Z
V	-0.0695644816981439	0.0296535947419484	0.1007505697185900
V	0.4899462304748662	0.0448036943954664	0.0980842571693720
V	0.0057766364307580	0.4975931923510243	0.0992345172869392
V	0.4827248621847122	0.4689366331731455	0.0971407510533150
Te	0.3194534072445042	0.3430037612406338	0.9901610786722219
Te	0.1621475236027806	0.1494548879626679	0.2065731565449845
Te	0.8146179589512736	0.3435620074750022	0.0038004077504968
Te	0.6334879767879894	0.1867242059629720	0.2104907044360134
Te	0.3035583045078938	0.8493424699041855	0.0175484241020698
Te	0.1513744115320400	0.6926218076684745	0.2071897978530324
Te	0.8071856434321157	0.8390028980540424	0.0007263678814257
Te	0.6173364453809876	0.6961974750570115	0.1871683216402104
Ru	0.9587049961825279	0.5173333338468749	0.2529416738538546

Table S8. Coordinates for the Y-doped system.

	X	Y	Z
V	-0.0356194629145022	0.0040492988510370	0.1053644862892512
V	0.5079688926648104	0.0635383979695588	0.0921292942567074
V	0.0097051389607546	0.5274949926809652	0.0966612845804295
V	0.4662180345473656	0.4949261404856612	0.1032128759828463
Te	0.3114318694793285	0.3659842671722137	0.9916321580044163

Te	0.1784027524635220	0.1567868436396311	0.1844885918692294
Te	0.8202667108754131	0.3526793417101084	0.0106405708046598
Te	0.6535049032461047	0.1857256726190534	0.2181202762695050
Te	0.3147405636117882	0.8568224061148324	0.0117327521947256
Te	0.1413186594379893	0.6774930343992995	0.2082337832112341
Te	0.8271827347384121	0.8463807011712425	-0.0029796924839210
Te	0.6264399280880197	0.7128751230981695	0.1751060905184755
Y	0.8551891898152992	0.4134737419216760	0.2774675564649671