Supporting Information

Understanding the Self-Healing Hydrophobic Recovery of High-Voltage Insulators

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The following tables contain force field data as implemented with LAMMPS code and based on the work found in Reference 30. C1 is a methyl carbon and also an oxidized carbon. C2 is a vinyl carbon used for termination of PDMS molecules. OW and HW are oxygen and hydrogen as part of water molecules.

Table 1: Atomic Masses

Atom	Mass [amu]
Si	15.999400
O	28.086000
C1	12.011150
H	1.007970
C2	12.011150
OW	15.9994
HW	1.008

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Table 2: Non-bonded Interactions

Atom	ε_{ij} [kcal/mol]	σ_{ij} [Å]
Si	0.2010230000	2.8461300000
O	0.2467760000	3.8504000000
C1	0.0979238000	3.4309000000
H	0.0099402300	2.9945200000
C2	0.0979238000	3.4309000000
OW	0.1550	3.1536
HW	0.0	0.0

Table 3: Bond Coefficients

Atoms	Force field	r_0 [Å]	K2 [kcal/mol Å^{-2}]	K3 [kcal/mol Å^{-3}]	K4 [kcal/mol Å^{-4}]
O–Si	class2	1.651	350.	-517.	674.
Si–C1	class2	1.878	190.	-279.	308.
Si–C2	class2	1.878	190.	-279.	308.
Atoms	Force field type	r_0 [Å]	K [kcal/mol Å^{-2}]		
C1–H	harmonic	1.092	328.		
C2–C2	harmonic	1.330	322.7158		
H–C2	harmonic	1.092	328.		
Si–H	harmonic	1.382	222.4		
C1–O	harmonic	1.3	615.3220		
OW–HW	harmonic	0.9572	1000.00		

Table 4: Angle Coefficients

Atoms	Force field	θ_0 [degrees]	K2 [kcal/mol radian^{-2}]	K3 [kcal/mol radian^{-3}]	K4 [kcal/mol radian^{-4}]
Si–O–Si	class2	137.63	10.305	-18.101	10.1
O–Si–C1	class2	109.82	23.022	-31.399	24.981
O –Si–C2	class2	109.82	23.022	-31.399	24.981
C1–Si–C1	class2	112.44	36.21	-20.39	20.02
C1 –Si–C2	class2	112.44	36.21	-20.39	20.02
Si –C1–H	class2	111.09	28.77	-13.95	0.0

Atoms	Force field	θ_0 [degrees]	K [kcal/mol radian^{-2}]
H–C1–H	harmonic	107.77	38.5
Si–C2–C2	harmonic	120.0	44.4
Si–C2–H	harmonic	120.0	44.4
H–C2–C2	harmonic	120.0	44.4
H–C2–H	harmonic	120.0	44.4
O–Si–O	harmonic	105.56	91.835
O–Si–H	harmonic	113.4	33.3
C1–Si–H	harmonic	109.1	32.7
Si–C1 –O	harmonic	120.0	70.0
O–C1–O	harmonic	120.0	70.0
HW–OW–HW	harmonic	104.52	100.0

Table 5: Dihedral Coefficients

Atoms	Force field	K1 [kcal/mol]	ϕ_1 [degrees]	K2 [kcal/mol]	ϕ_2 [degrees]	K3 [kcal/mol]	ϕ_3 [degrees]	θ^0_{ijk}	n
Si–O –Si–C1	class2_dl	0	180.	0	180.	0.02853	180.	146.	2
Si –O–Si–C2	class2_dl	0	180.	0	180.	0.02853	180.	146.	2
Si –O–Si–O	class2_dl	0.205	180.	-0.1365	180.	-0.1098	180.	146.	2
O–Si–C1–H	class2	0	180.	0	180.	0.075	180.		
C1–Si–C1–H	class2	0	180.	0	180.	0.075	180.		
C2–Si–C1–H	class2	0	180.	0	180.	0.075	180.		
O–Si–C2–C2	class2	0	180.	0	180.	0.075	180.		
O–Si –C2–H	class2	0	180.	0	180.	0.075	180.		
C1–Si–C2–C2	class2	0	180.	0	180.	0.075	180.		
C1–Si–C2–H	class2	0	180.	0	180.	0.075	180		
Si–O–Si–H	class2_dl	0	180.	0	180.	0.02853	180.	146.	2
H–Si–C1–H	class2	0	180.	0	180.	0.075	180.		
O–Si–C1–H	class2	0	180.	0	180.	0.075	180.		
C1–Si–C1–H	class2	0	180.	0	180.	0.075	180.		

Atoms	Force field	K [kcal/mol]	d	n
Si–C2–C2–H	harmonic	-0.3000	1	2
H–C2–C2–H	harmonic	-0.3000	1	2

Table 6: Improper Coefficients

Atoms	K [kcal/mol radian^{-2}]	χ_0 [degrees]
Si–C2–H–C2	20.0	180.
H–C2–H–C2	20.0	180.