Electronic Supplementary Information

Electron delocalization in defected graphene and its ability to the tetrel bonds formation

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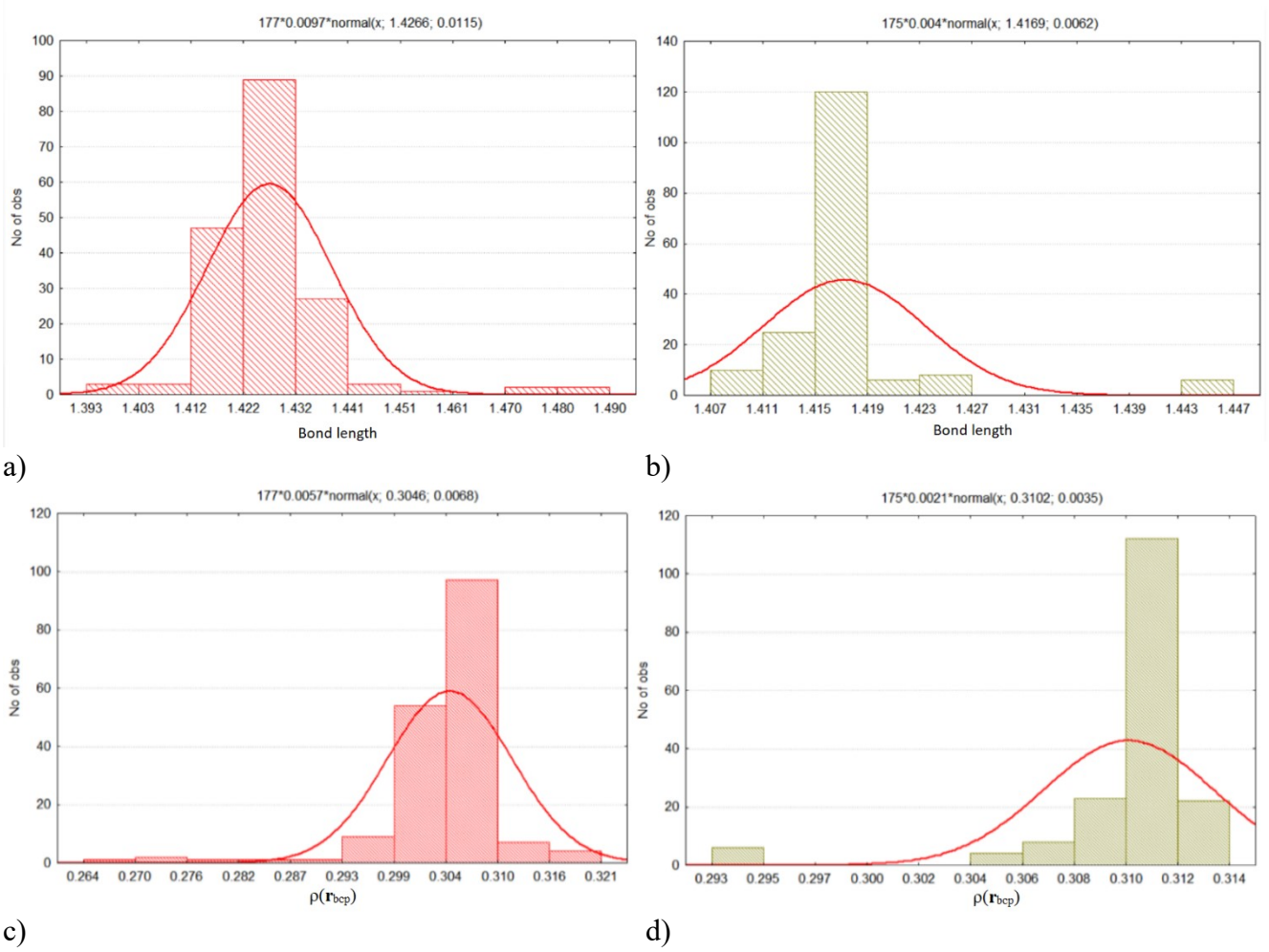
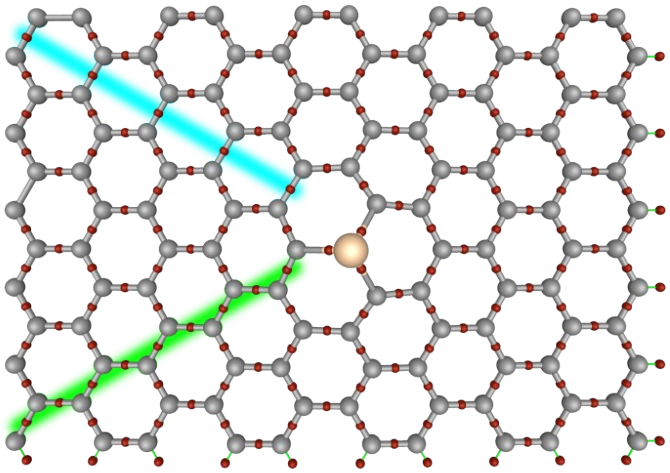
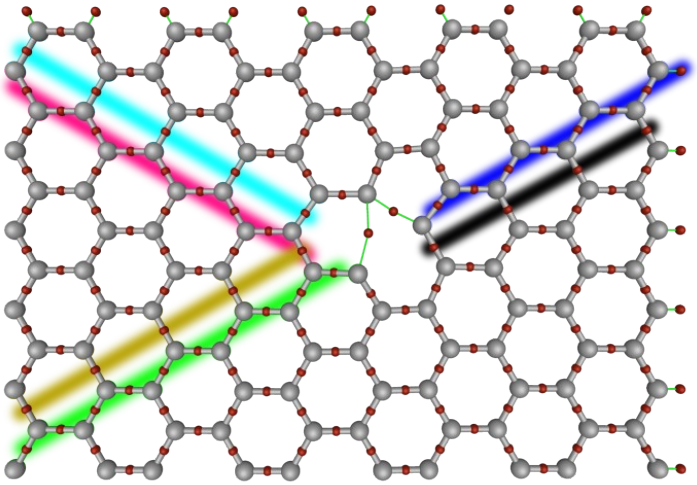


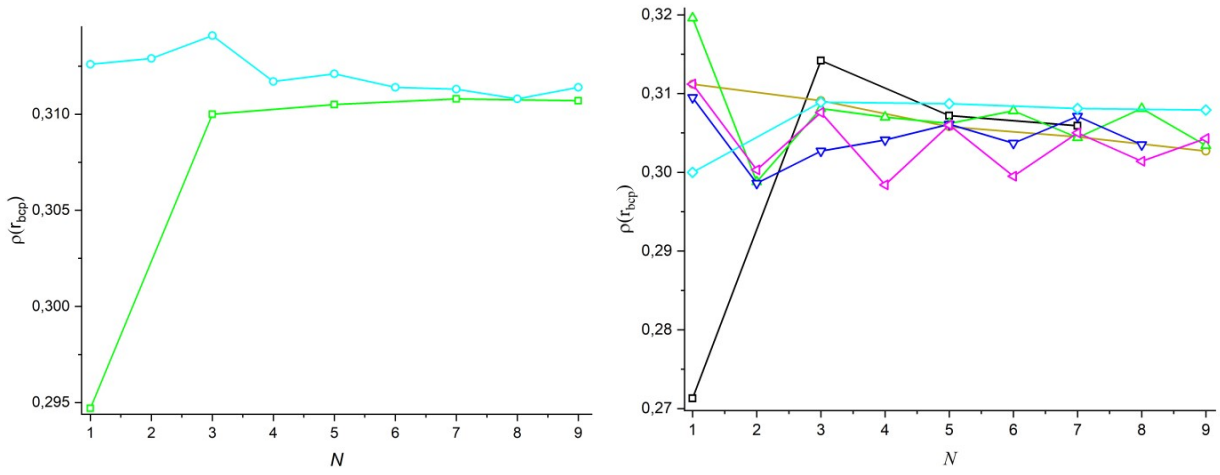
Figure S1. Histograms showing the C_g–C_g bond length distribution and distribution of electron density at bcp for C_g–C_g bonds a,c) in graphene with a vacancy b,d) in graphene with Si-defect



a)



b)



c) d)

Figure S2. Scheme of directions in defected graphene for analysis of defect influence on electron density distribution at bcp of the ordinary C_g–C_g bonds a) in Si-defected layer and b) in vacancy-defected graphene. Electron density at bond critical points moving away from a defect in various directions c) in Si-defected layer and d) in vacancy-defected graphene

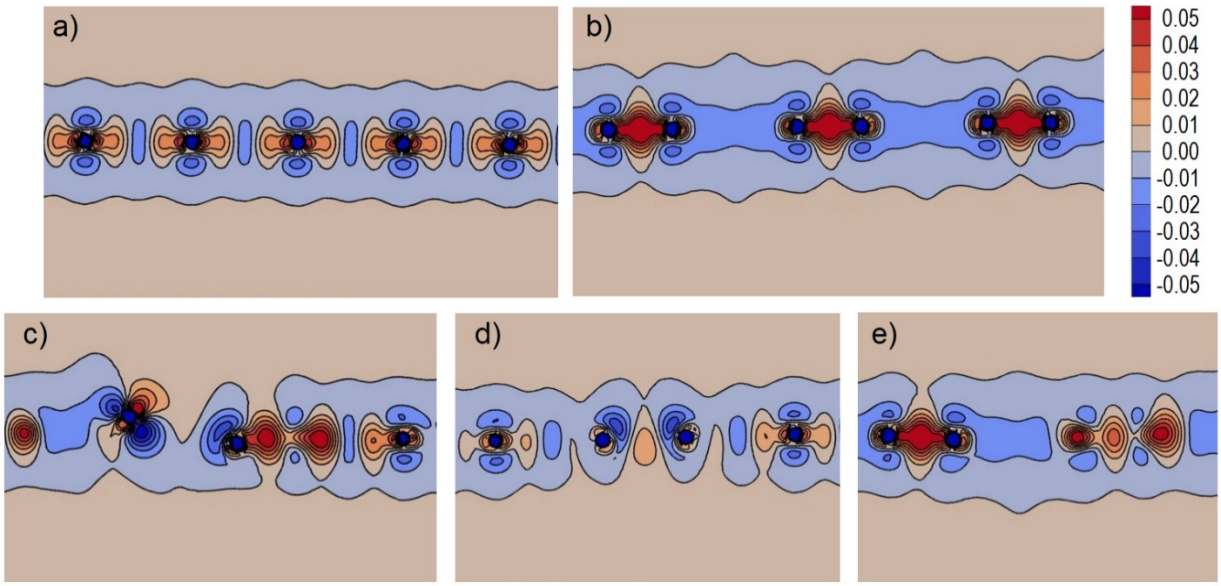


Figure S3. Deformation density, $\delta\rho(\mathbf{r})$, in planes perpendicular to graphene layer for the defect-free graphene (a,b) and for the graphene with a vacancy (c,d,e). Planes b) and e) contain C_g–C_g covalent bonds, which in the case of defected graphene belongs to the vacancy edge (i.e. C_g^2–C_g^3 bond, see Fig. 3a). Planes c), d) contain $C_g^1 \ldots C_g^5$ and $C_g^5 \ldots C_g^9$ noncovalent bonds in the vacancy region (Fig. 3a), while plane (a) corresponds to the similar plane in defect-free graphene.

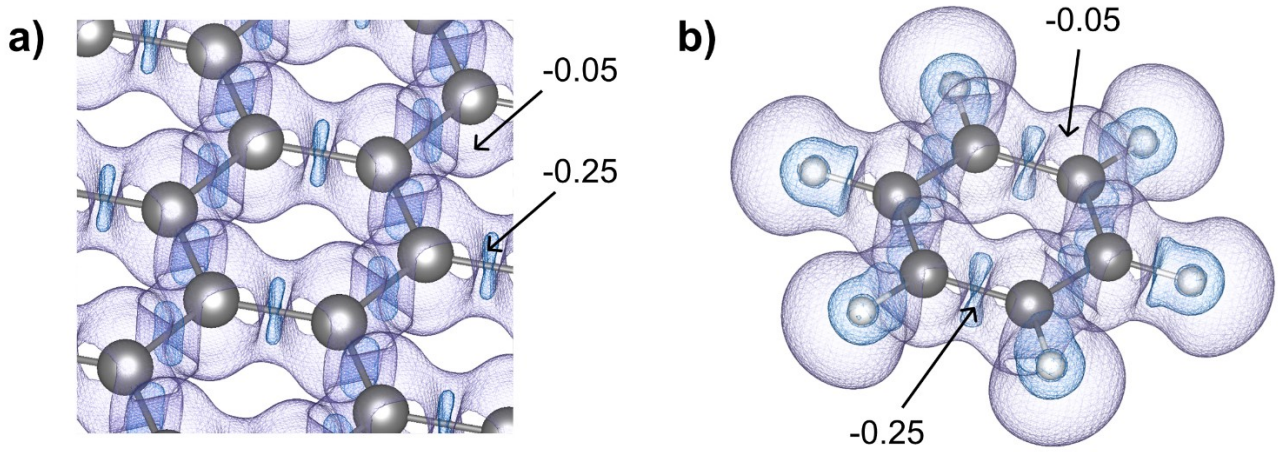


Figure S4. The fermionic potential, $v_f(r)$, distribution in the defect-free graphene (a) and benzene molecule (b). The values of the depicted isosurfaces are given in the a.u.

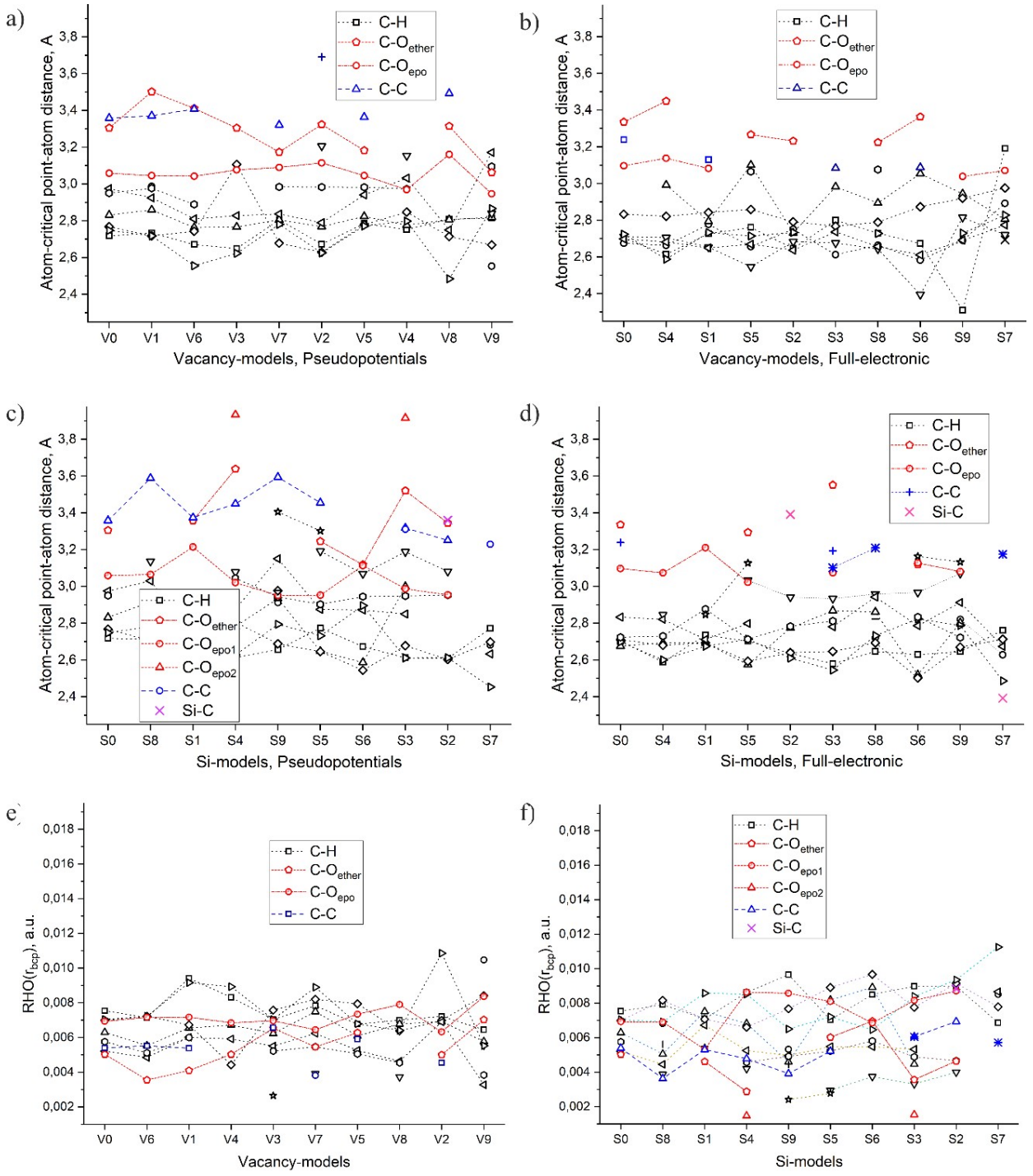
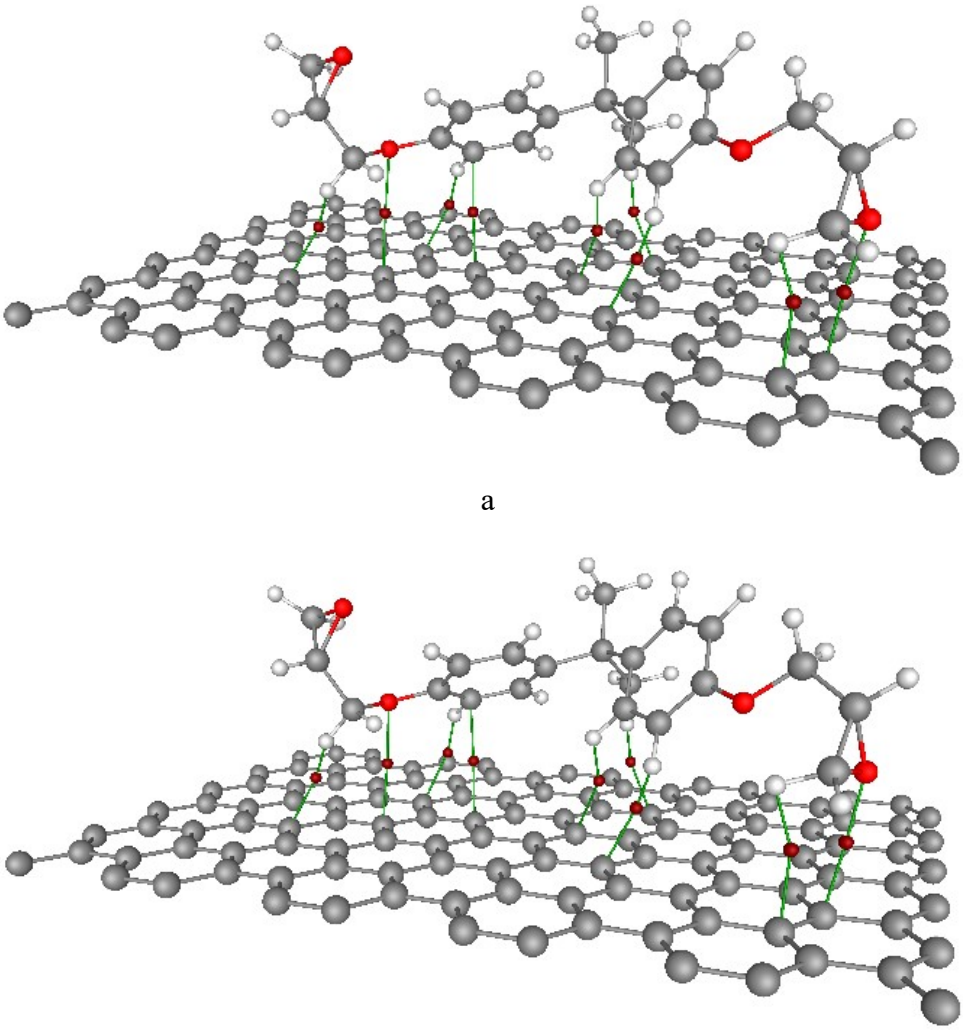


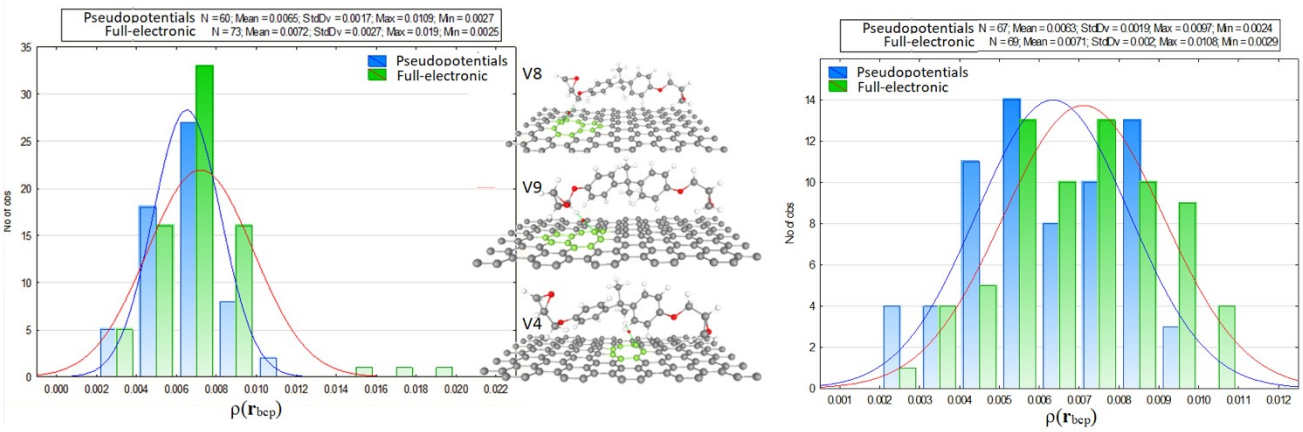
Figure S5. Interatomic distances for noncovalent bonds in the systems ranked by E_{int} "DGEBA – vacancy-defected graphene": a) pseudopotential basis sets; b) full-electron basis sets; "DGEBA – Si-defected graphene": c) pseudopotential basis sets; d) full-electron basis sets. Electron density at bcp of noncovalent bonds calculated in pseudopotential basis sets: e) vacancy-defected models; f) Si-defected models



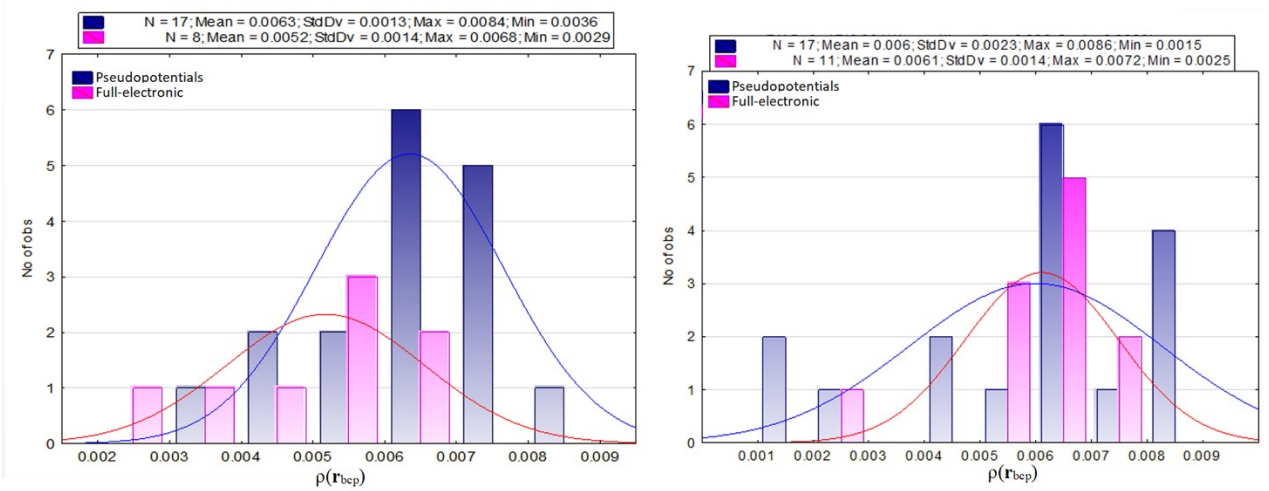
a

b

Figure S6. Bond paths for interactions of DGEBA and defect-free graphene C_g atoms according to a) full-electron computation; b) pseudopotential computation



a) b)



c) d)

Figure S7. Distributions of the values of electron density at bcp C_g…H a) for the graphene-DGEBA models with vacancy (three relatively strongest bonds formed by CH_2 or CH_3 groups DGEBA with C_g belonging to the edge of defect are in the right); b) for models with Si-defect. Distributions of electron density at bcp for C^g…O bonds: c) in systems "DGEBA – graphene with vacancy"; d) in systems "DGEBA – graphene with Si-defect"

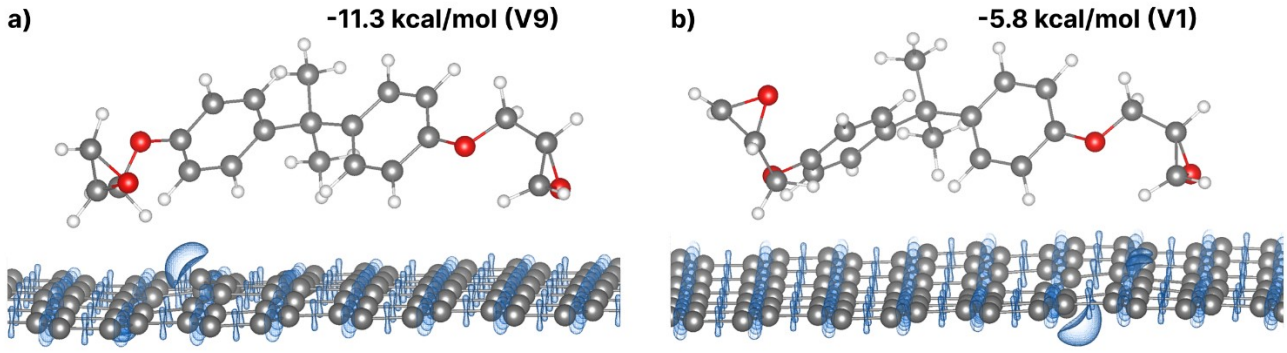
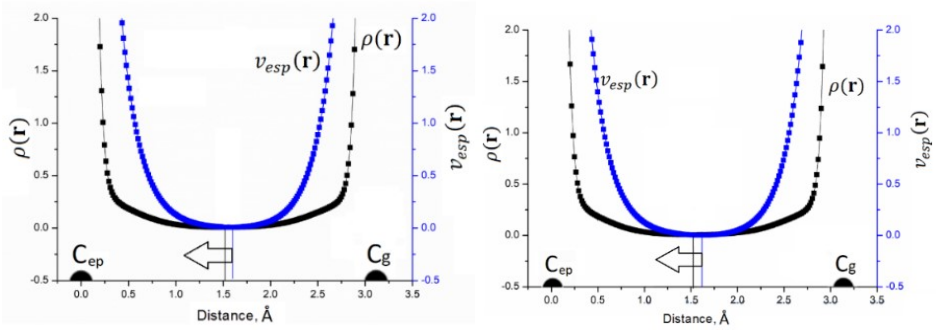


Figure S8. The fermionic potential, $v_f(r)$, distribution (-0.25 a.u.) in the graphene layer of the graphene-DGEBA systems with a vacancy (V9 and V1 systems). The ΔE_{int} = E_{int}(system) – E_{int}(ideal graphene) is shown on the each frame.



a) b)

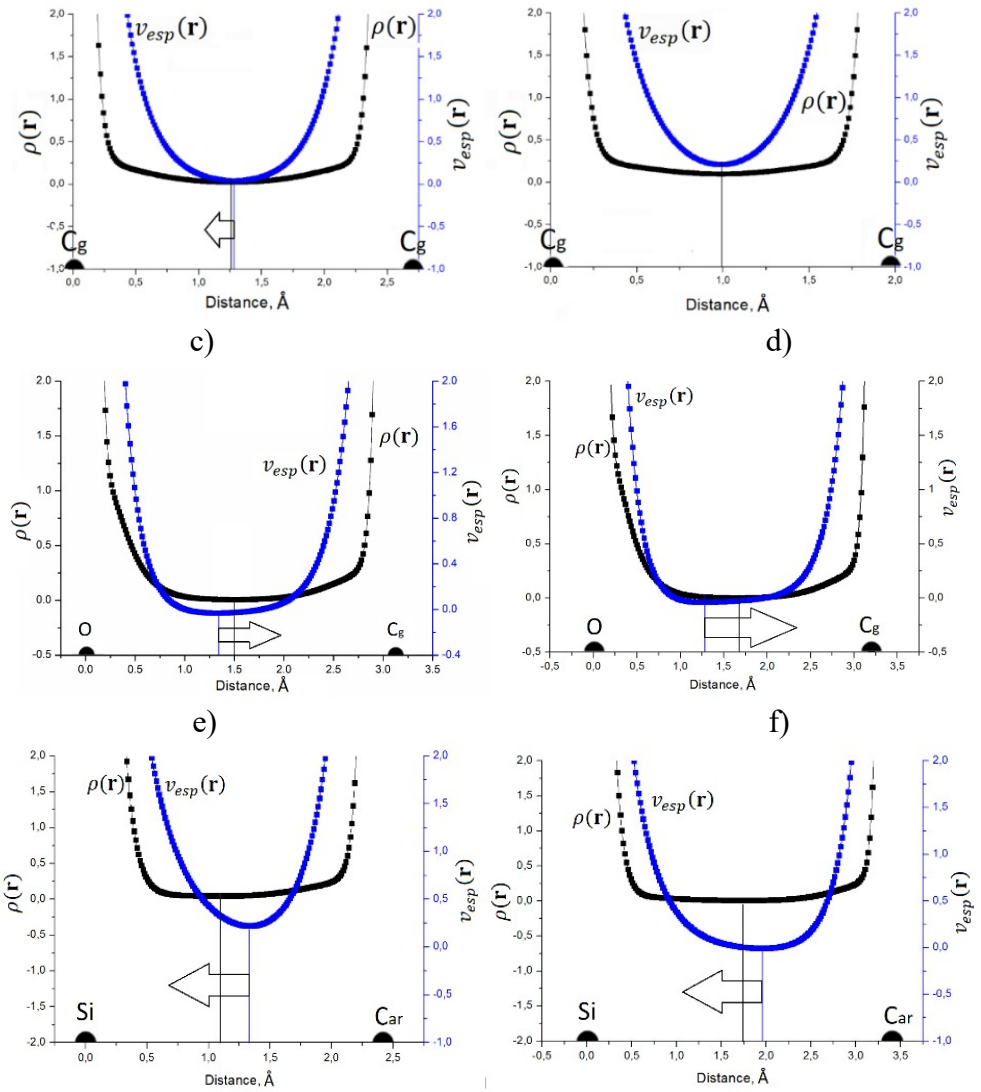


Figure S9. Superposition of the boundaries of atomic basins in electrostatic potential and electron density along the line of a) C_g …C_{ep} interaction (C_{ep} in DGEBA near the epoxy O) in V4 model; b) C_g …C_{ep} interaction (C_{ep} in DGEBA near the epoxy O) in S7 model; c) the polar intralayer C_g…C_g bond for graphene with the vacancy; d) the nonpolar intralayer C_g…C_g bond for graphene with the vacancy; e) tetrel bond C_g…O (epoxy oxygen) for DGEBA and defected-free graphene; f) tetrel bond C_g…O (ether oxygen) for DGEBA and defected-free graphene; g) relatively strong Si…C_g interaction in Si-defect (S7 model); h) weak Si…C_g interaction in Si-defect (S2 model).

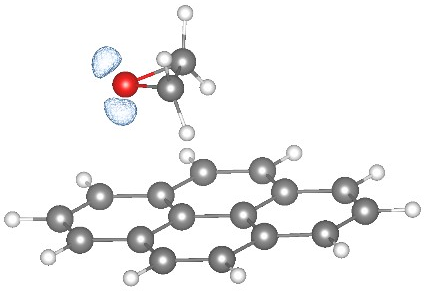


Figure S10. Fermionic potential -0.200 a.u. isosurface for the O atom in the isolated complex of ethylene oxide and four condensed benzene rings.

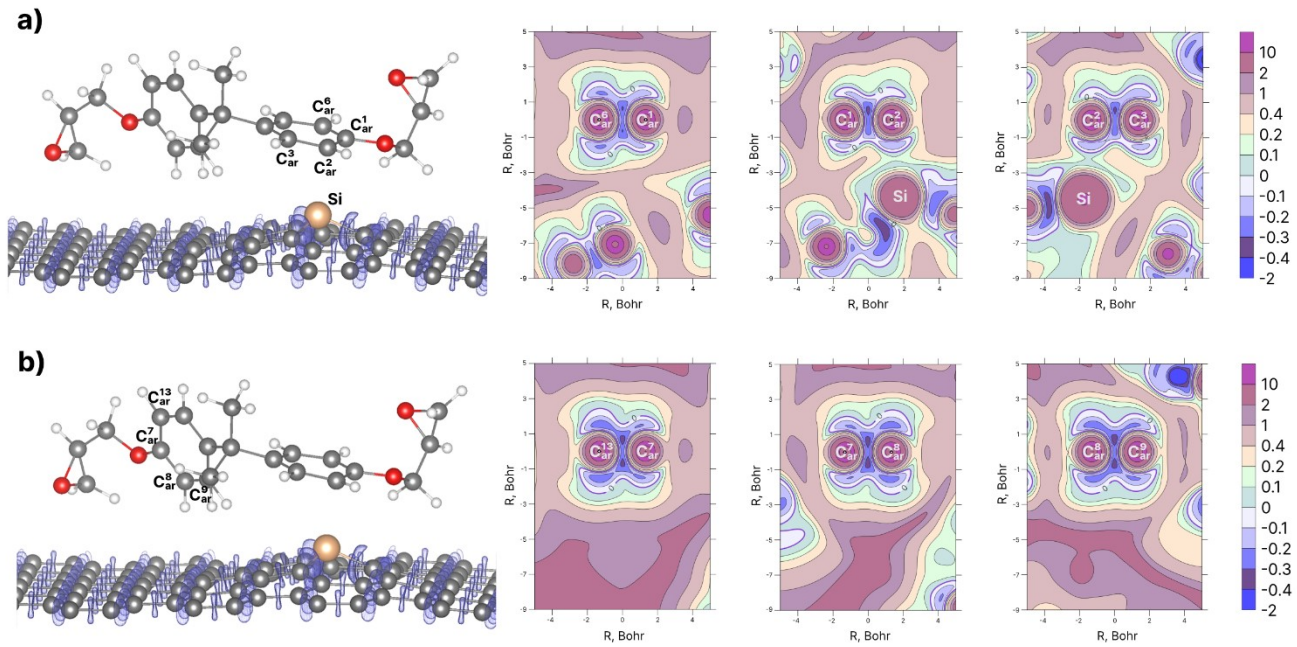


Figure S11. The fermionic potential, $v_f(r)$, in the graphene-DGEBA system (model S7). 3D distribution is shown only for the graphene layer (-0.25 a.u. isosurface), while 2D maps are depicted $v_f(r)$ in the planes of the DGEBA aryl rings. All of them include C_{ar}–C_{ar} bonds and are orthogonal to the plane of the corresponding aryl ring.

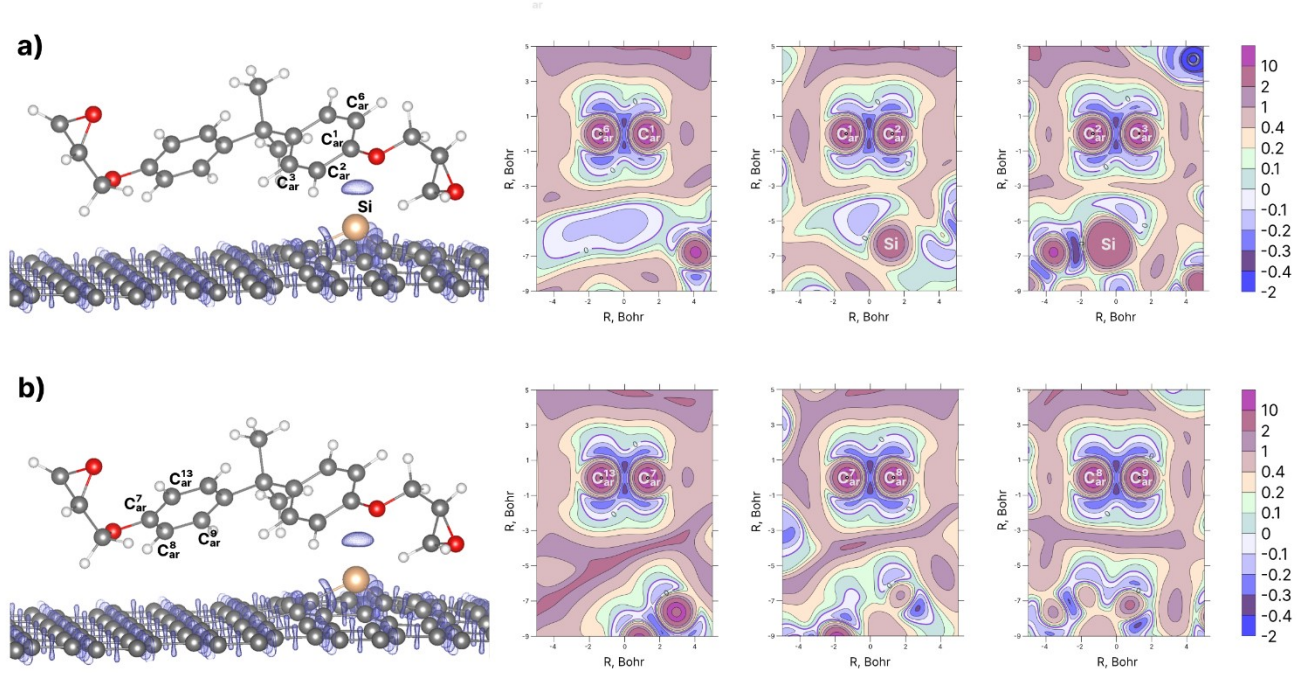


Figure S12. The fermionic potential, $v_f(r)$, in the graphene-DGEBA system (model S2). 3D distribution is shown only for the graphene layer (-0.25 a.u. isosurface), while 2D maps are depicted $v_f(r)$ in the planes of the DGEBA aryl rings. All of them include C_{ar}–C_{ar} bonds and are orthogonal to the plane of the corresponding aryl ring.

Table S1. The relative energy (E_{rel}, kcal/mol) and the interaction energy (E_{int}, kcal/mol) for the systems of DGEBA and graphene with a vacancy (V-models), and with a Si-defect (S-models).

	E_{rel}	E_{int}	E_{int} +BSSE	E_{int} noRelax +BSSE	E_{int} noRelax	E_{rel}	E_{int}
	Pseudopotential calculations					Full-electronic calculations	
Defect-free	-	-35.1	-25.9	-26.6	-35.7	-	-13.7
V1	3.9	-34.4	-25.2	-26.2	-35.3	5.5	-19.5
V2	3.0	-35.3	-25.7	-26.5	-36.1	4.4	-20.5
V3	3.3	-34.9	-25.3	-26.5	-36.1	5.1	-19.8
V4	3.5	-34.8	-25.7	-26.4	-35.6	3.7	-21.3
V5	3.1	-35.2	-25.7	-26.8	-36.3	4.2	-20.8
V6	4.0	-34.3	-25.0	-26.5	-35.8	5.2	-19.8
V7	3.3	-35.0	-25.6	-26.6	-36.1	4.7	-20.2
V8	3.0	-35.3	-26.2	-27.1	-36.1	2.2	-22.8
V9	0.0	-38.3	-27.8	-28.8	-39.2	0.0	-25.0
S1	8.3	-35.2	-25.8	-26.1	-35.4	5.6	-20.3
S2	5.1	-38.3	-27.7	-29.6	-40.2	4.1	-21.7
S3	5.7	-37.8	-27.9	-28.2	-38.1	4.1	-21.8
S4	8.0	-35.5	-26.4	-26.9	-36.0	6.2	-19.7
S5	6.5	-36.9	-27.3	-27.7	-37.3	4.8	-21.1
S6	6.3	-37.2	-27.4	-27.7	-37.5	3.7	-22.2
S7	0.0	-43.4	-32.6	-39.0	-49.8	0.0	-25.8
S8	8.4	-35.0	-25.4	-27.6	-37.2	3.7	-22.2
S9	6.6	-36.8	-26.8	-28.4	-38.4	3.6	-22.3

Table S2. The bond length and the properties of electron density at the bond critical points for noncovalent bonds in the systems of DGEBA and graphene with a vacancy. (The bonds in italics refer to intralayer bonds).

Model	Noncovalent bond	Bond Length, Å	Electron density, ρ(rbcp), a.u.	Laplacian of electron density, ∇2ρ(rbcp), a.u.	Kinetic energy density, g(rbcp), a.u.	Potential energy density, v(rbcp), a.u.
V1	H10...C66	2.663	0.008	0.029	0.006	-0.004
	C86...O166	3.449	0.003	0.017	0.003	-0.002
	H17...C105	2.615	0.009	0.032	0.007	-0.005
	H5...C58	2.992	0.004	0.018	0.003	-0.002
	H6...C59	2.706	0.007	0.026	0.005	-0.004
	H4...C80	2.822	0.006	0.023	0.004	-0.003
	H9...C81	2.682	0.008	0.028	0.006	-0.004
	H22...C91	2.588	0.009	0.035	0.007	-0.005
	C83...O167	3.138	0.006	0.026	0.005	-0.004
	C91...C101	2.481	0.033	0.066	0.016	-0.016
	C91...C110	1.893	0.119	-0.088	0.027	-0.076

	C101...C110	2.496	0.032	0.066	0.016	-0.015
V2	H17...C85	2.800	0.006	0.025	0.005	-0.003
	H10...C57	2.612	0.009	0.033	0.007	-0.005
	H17...C86	2.809	0.006	0.028	0.005	-0.004
	H5...C47	2.982	0.004	0.017	0.003	-0.002
	H6...C59	2.677	0.008	0.026	0.005	-0.004
	H4...C79	2.767	0.006	0.023	0.004	-0.003
	H9...C89	2.737	0.007	0.024	0.005	-0.003
	C110...C163	3.084	0.008	0.034	0.007	-0.005
	C81...C100	1.883	0.121	-0.097	0.027	-0.079
	C81...C89	2.495	0.032	0.067	0.016	-0.015
	C100...C89	2.487	0.032	0.067	0.016	-0.016
V3	H17...C95	2.761	0.007	0.025	0.005	-0.004
	C85...O166	3.267	0.005	0.024	0.005	-0.003
	H10...C57	2.656	0.008	0.030	0.006	-0.005
	H5...C48	3.101	0.003	0.013	0.002	-0.001
	H6...C60	2.547	0.010	0.030	0.006	-0.005
	H4...C88	2.859	0.005	0.023	0.004	-0.003
	H9...C99	2.670	0.008	0.031	0.006	-0.005
	H22...C121	2.714	0.008	0.032	0.006	-0.004
	H21...C131	3.065	0.003	0.015	0.003	-0.002
	C69...C88	1.870	0.124	-0.108	0.028	-0.083
	C69...C79	2.494	0.032	0.067	0.016	-0.015
	C88...C79	2.483	0.033	0.067	0.016	-0.016
V4	H17...C95	2.673	0.008	0.028	0.006	-0.004
	C85...O166	3.363	0.004	0.021	0.004	-0.003
	H10...C65	2.582	0.009	0.034	0.007	-0.005
	H5...C58	3.054	0.004	0.017	0.003	-0.002
	H4...C78	2.873	0.005	0.021	0.004	-0.003
	H6...C59	2.395	0.016	0.038	0.009	-0.009
	H9...C88	2.611	0.009	0.033	0.007	-0.005
	C163...C110	3.087	0.007	0.032	0.006	-0.005
	C59...C48	2.507	0.031	0.066	0.016	-0.015
	C67...C48	1.885	0.122	-0.099	0.027	-0.079
	C59...C67	2.506	0.031	0.066	0.016	-0.015
V5	H17...C95	2.729	0.007	0.026	0.005	-0.004
	C85...O166	3.224	0.005	0.025	0.005	-0.004
	H10...C57	2.664	0.008	0.029	0.006	-0.004
	C77...C152	3.241	0.006	0.027	0.005	-0.003
	H5...C48	2.894	0.005	0.019	0.003	-0.002
	H4...C78	2.790	0.006	0.023	0.004	-0.003
	H6...C59	2.643	0.009	0.029	0.006	-0.005
	H9...C99	2.657	0.008	0.030	0.006	-0.004
	H22...C121	2.728	0.007	0.032	0.006	-0.004
	H21...C131	3.077	0.003	0.015	0.003	-0.002
	C59...C78	1.869	0.125	-0.109	0.028	-0.083

	C59...C67	2.484	0.033	0.067	0.016	-0.016
	C78...C67	2.485	0.033	0.067	0.016	-0.016
V6	H17...C95	2.726	0.007	0.026	0.005	-0.004
	H10...C66	2.778	0.006	0.026	0.005	-0.003
	H18...C96	2.866	0.005	0.024	0.004	-0.003
	C152...C77	3.129	0.007	0.030	0.006	-0.004
	H5...C58	2.794	0.006	0.025	0.005	-0.003
	H4...C87	2.842	0.005	0.019	0.004	-0.002
	H6...C59	2.653	0.008	0.030	0.006	-0.005
	H9...C99	2.649	0.008	0.030	0.006	-0.005
	H22...C121	2.733	0.007	0.032	0.006	-0.004
	C110...O167	3.082	0.007	0.032	0.006	-0.005
	C58...C67	2.490	0.032	0.067	0.016	-0.015
	C58...C77	1.872	0.124	-0.107	0.028	-0.082
	C67...C77	2.487	0.032	0.067	0.016	-0.016
V7	H17...C104	2.647	0.008	0.031	0.006	-0.005
	O166...C105	3.232	0.005	0.026	0.005	-0.004
	H10...C85	2.751	0.007	0.027	0.005	-0.004
	H5...C67	2.731	0.007	0.028	0.005	-0.004
	H4...C87	2.792	0.006	0.022	0.004	-0.003
	H6...C68	2.683	0.008	0.026	0.005	-0.004
	H9...C99	2.637	0.009	0.031	0.006	-0.005
	H22...C121	2.734	0.007	0.031	0.006	-0.004
	C67...C86	1.868	0.125	-0.111	0.028	-0.084
	C67...C77	2.485	0.033	0.067	0.016	-0.016
	C77...C86	2.488	0.032	0.067	0.016	-0.015
V8	H17...C85	2.311	0.019	0.042	0.011	-0.012
	H10...C57	2.690	0.008	0.029	0.006	-0.004
	H5...C47	2.945	0.004	0.018	0.003	-0.002
	H6...C40	2.816	0.006	0.024	0.005	-0.003
	H4...C69	2.920	0.005	0.023	0.004	-0.003
	H9...C89	2.691	0.008	0.027	0.005	-0.004
	H22...C101	2.730	0.007	0.028	0.005	-0.004
	O167...C91	3.039	0.007	0.031	0.006	-0.005
	C77...C96	1.892	0.120	-0.095	0.026	-0.077
	C77...C85	2.518	0.030	0.066	0.015	-0.014
	C96...C85	2.511	0.030	0.067	0.016	-0.015
V9	H4...C98	2.968	0.004	0.017	0.003	-0.002
	H5...C67	2.804	0.006	0.021	0.004	-0.003
	H6...C79	2.697	0.008	0.028	0.006	-0.004
	H9...C108	2.763	0.007	0.025	0.005	-0.003
	H10...C77	2.848	0.005	0.021	0.004	-0.003
	H17...C85	3.180	0.003	0.012	0.002	-0.001
	H18...C97	2.380	0.016	0.038	0.010	-0.010
	H20...C104	2.642	0.009	0.030	0.006	-0.005
	H22...C110	2.812	0.007	0.029	0.006	-0.004

	O167...C111	3.068	0.007	0.031	0.006	-0.005
	C86...C97	2.508	0.030	0.066	0.016	-0.015
	C86...C105	1.887	0.121	-0.097	0.027	-0.078

Table S3. The bond length and the properties of electron density at the bond critical points for noncovalent bonds in the systems of DGEBA and Si-defected graphene.

Model	Noncovalent bond	Bond Length, Å	Electron density, $\rho(\mathbf{r}_{bcp})$, a.u.	Laplacian of electron density, $\nabla^2\rho(\mathbf{r}_{bcp})$, a.u.	Kinetic energy density, $g(\mathbf{r}_{bcp})$, a.u.	Potential energy density, $v(\mathbf{r}_{bcp})$, a.u.
S1	H4...C79	2.702	0.0070	0.0247	0.0049	-0.0035
	H6...C59	2.681	0.0076	0.0247	0.0050	-0.0037
	H9...C89	2.608	0.0092	0.0322	0.0066	-0.0051
	H10...C66	2.645	0.0088	0.0316	0.0064	-0.0049
	H17...C85	2.726	0.0071	0.0271	0.0053	-0.0038
	H21...C132	2.862	0.0055	0.0223	0.0042	-0.0028
	C122...H22	2.808	0.0065	0.0290	0.0055	-0.0037
	C103...O168	3.192	0.0052	0.0245	0.0049	-0.0037
S2	H5...C68	2.942	0.0043	0.0185	0.0033	-0.0021
	H6...C80	2.640	0.0091	0.0288	0.0059	-0.0047
	H9...C109	2.610	0.0088	0.0335	0.0066	-0.0049
	H10...C78	2.774	0.0073	0.0321	0.0061	-0.0041
	H17...C96	2.636	0.0089	0.0300	0.0061	-0.0048
	H22...C130	2.783	0.0064	0.0247	0.0047	-0.0032
	SI90...C152	3.391	0.0088	0.0208	0.0046	-0.0039
	C122...O168	3.049	0.0073	0.0318	0.0066	-0.0053
S3	H4...C88	2.781	0.0059	0.0214	0.0041	-0.0028
	H5...C57	2.911	0.0047	0.0188	0.0034	-0.0022
	H6...C67	2.634	0.0086	0.0299	0.0061	-0.0047
	H9...C100	2.541	0.0098	0.0316	0.0066	-0.0054
	H10...C76	2.817	0.0060	0.0236	0.0045	-0.0031
	H17...C105	2.572	0.0095	0.0334	0.0068	-0.0053
	C164...C111	3.093	0.0072	0.0325	0.0063	-0.0045
	H22...C121	2.802	0.0060	0.0244	0.0046	-0.0031
	C77...C153	3.158	0.0071	0.0318	0.0061	-0.0042
	C96...O167	3.543	0.0024	0.0154	0.0028	-0.0017
	C102...O168	3.065	0.0071	0.0319	0.0066	-0.0053
S4	H4...C88	2.905	0.0047	0.0181	0.0033	-0.0022
	H5...C58	2.943	0.0044	0.0185	0.0034	-0.0021
	H6...C69	2.636	0.0088	0.0349	0.0070	-0.0052
	H7...C48	3.202	0.0028	0.0111	0.0020	-0.0011
	H9...C100	2.736	0.0072	0.0268	0.0052	-0.0038
	H10...C66	2.585	0.0094	0.0339	0.0069	-0.0053
	H17...C85	2.683	0.0079	0.0281	0.0056	-0.0042
	H18...C97	2.973	0.0043	0.0196	0.0036	-0.0023
	H22...C122	2.743	0.0070	0.0298	0.0056	-0.0038

	O168...C112	3.023	0.0075	0.0324	0.0067	-0.0054
S5	H4...C89	2.778	0.006	0.024	0.004	-0.003
	H5...C48	3.024	0.003	0.014	0.002	-0.001
	H6...C60	2.581	0.010	0.034	0.007	-0.006
	H9...C101	2.674	0.008	0.030	0.006	-0.004
	H10...C57	2.581	0.010	0.035	0.007	-0.006
	H17...C86	2.687	0.008	0.031	0.006	-0.004
	H21...C132	3.092	0.003	0.015	0.003	-0.002
	H22...C122	2.701	0.007	0.029	0.005	-0.004
	C77...O167	3.215	0.006	0.026	0.005	-0.004
	O168...C112	3.018	0.007	0.031	0.006	-0.005
S6	H4...C80	2.781	0.006	0.023	0.004	-0.003
	H5...C48	2.962	0.004	0.016	0.003	-0.002
	H6...C60	2.513	0.011	0.034	0.007	-0.006
	H9...C89	2.802	0.006	0.028	0.005	-0.004
	H10...C57	2.519	0.011	0.034	0.007	-0.006
	H17...C85	2.598	0.009	0.033	0.007	-0.005
	O167...C86	3.114	0.007	0.029	0.006	-0.005
	H22...C122	2.718	0.008	0.032	0.006	-0.004
	O168...C111	3.101	0.007	0.032	0.006	-0.005
S7	H4...C99	2.651	0.009	0.029	0.006	-0.005
	H6...C79	2.698	0.008	0.025	0.005	-0.004
	H9...C109	2.486	0.011	0.035	0.008	-0.006
	SI78...C153	2.392	0.046	-0.005	0.013	-0.027
	H17...C85	2.754	0.007	0.026	0.005	-0.003
	H18...C97	2.625	0.009	0.032	0.006	-0.005
	C164...C131	3.116	0.007	0.030	0.006	-0.004
S8	H4...C80	2.900	0.005	0.020	0.004	-0.002
	H5...C67	2.955	0.005	0.022	0.004	-0.003
	H6...C59	2.651	0.009	0.029	0.006	-0.005
	H9...C100	2.709	0.008	0.030	0.006	-0.004
	H10...C66	2.810	0.006	0.022	0.004	-0.003
	H17...C96	2.611	0.009	0.031	0.006	-0.005
	H18...C97	2.695	0.008	0.030	0.006	-0.004
	H20...C117	2.838	0.005	0.023	0.004	-0.003
	H22...C122	2.754	0.007	0.032	0.006	-0.004
S9	H4...C80	2.872	0.005	0.022	0.004	-0.003
	H5...C67	3.034	0.004	0.019	0.003	-0.002
	H6...C60	2.671	0.008	0.028	0.006	-0.004
	H9...C110	2.762	0.007	0.024	0.005	-0.003
	H10...C66	2.785	0.006	0.023	0.004	-0.003
	H17...C85	2.626	0.009	0.032	0.007	-0.005
	H18...C98	2.809	0.006	0.021	0.004	-0.003
	H20...C126	2.770	0.006	0.023	0.004	-0.003
	H21...C132	3.088	0.003	0.015	0.003	-0.002
	O168...C112	3.069	0.007	0.031	0.006	-0.005

	H22...C122	2.695	0.008	0.031	0.006	-0.004

Table S4. Visual analysis of the mutual orientations for lone electron pairs (LP) of ether (O_{et}) and epoxy (O_{ep}) oxygen, centres of (C_g–C_g) bonds, areas above C_g atoms in the π-plane, π(C_g), ring critical points (rcp) in the systems of DGEBA and defected graphene

Model	Noncovalent bond	Types of orientation		
V1	C86...O166	$O_{et} \leftrightarrow C_g$-$C_g$	LP(O_{et}) $\leftrightarrow$ C_g-C_g	
V1	C83...O167	$O_{ep} \leftrightarrow C_g$-$C_g$	LP(O_{ep}) $\leftrightarrow$ ring	LP(O_{ep}) $\leftrightarrow$ ring*
V3	C85...O166	$O_{et} \leftrightarrow C_g$-$C_g$	LP(O_{et}) $\leftrightarrow$ rcp	
V4	C85...O166	$O_{et} \leftrightarrow C_g$-$C_g$	LP(O_{et}) $\leftrightarrow$ ring	
V5	C85...O166	$O_{et} \leftrightarrow$ π(C_g)	LP(O_{et}) $\leftrightarrow$ C_g-C_g	
V6	C110...O167	$O_{ep} \leftrightarrow$ ring (C_g)	LP(O_{ep}) $\leftrightarrow$ ring	LP(O_{ep}) $\leftrightarrow$ ring
V7	O166...C105	$O_{et} \leftrightarrow C_g$-$C_g$	LP(O_{et}) $\leftrightarrow$ rcp	
V8	O167...C91	$O_{ep} \leftrightarrow$ ring (C_g)	LP(O_{ep}) $\leftrightarrow$ C_g-C_g	LP(O_{ep}) $\leftrightarrow$ ring
V9	O167...C111	$O_{ep} \leftrightarrow$ ring (C_g)	LP(O_{ep}) $\leftrightarrow$ C_g-C_g	LP(O_{ep}) $\leftrightarrow$ ring
S1	C103...O168	$O_{ep} \leftrightarrow$ ring (C_g)	LP(O_{ep}) $\leftrightarrow$ C_g-C_g	LP(O_{ep}) $\leftrightarrow$ C_g-Si
S2	C122...O168	$O_{ep} \leftrightarrow$ ring (C_g)	LP(O_{ep}) $\leftrightarrow$ C_g-C_g	LP(O_{ep}) $\leftrightarrow$ π(C_g)
S3	C96...O167	$O_{et} \leftrightarrow$ rcp	LP(O_{et}) $\leftrightarrow$ rcp	
S3	C102...O168	$O_{ep} \leftrightarrow$ ring (C_g)	LP(O_{ep}) $\leftrightarrow$ rcp	LP(O_{ep}) $\leftrightarrow$ C_g-C_g
S4	O168...C112	$O_{ep} \leftrightarrow C_g$-$C_g$	LP(O_{ep}) $\leftrightarrow$ ring	LP(O_{ep}) $\leftrightarrow$ ring
S5	C77...O167	$O_{et} \leftrightarrow C_g$-$C_g$	LP(O_{et}) $\leftrightarrow$ rcp	
S5	O168...C112	$O_{ep} \leftrightarrow$ π(C_g)	LP(O_{ep}) $\leftrightarrow$ C_g-C_g	LP(O_{ep}) $\leftrightarrow$ rcp
S6	O167...C86	$O_{et} \leftrightarrow C_g$-$C_g$	LP(O_{et}) $\leftrightarrow$ rcp	
S6	O168...C111	$O_{ep} \leftrightarrow C_g$-$C_g$	LP(O_{ep}) $\leftrightarrow$ ring	LP(O_{ep}) $\leftrightarrow$ ring
S9	O168...C112	$O_{ep} \leftrightarrow C_g$-$C_g$	LP(O_{ep}) $\leftrightarrow$ C_g-C_g	LP(O_{ep}) $\leftrightarrow$ π(C_g)

*ring – the case when it is difficult to describe disposition of element, but it is obvious that it hangs near the area of graphene ring, not over the center.