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Supporting Information

SiG–pollutant systems in an aqueous environment

Table S1. Geometrical parameters of the SiG-pollutant systems with explicit $15 \cdot H_2O$ molecules, in addition to COSMO implicit solvent environment. Distances are in angstroms (Å).

Pollutant		$d_{Si\text{-}O1}$	$d_{As\text{-}O1}$	$d_{H\text{-}O1}$
SiG-MMA^{III}	a	1.74	2.27	1.04
	b	1.73	2.12	1.04
	c	1.73	2.18	1.04
SiG-DMA^{III}	a	1.71	2.37	1.02
	b	1.69	2.13	1.56
SiG-MMA^{V}	a	1.75	1.76	1.79
	b	1.75	1.77	1.88
	c	1.74	1.78	1.81
	d	1.77	1.78	1.88
	e	1.90	1.75	-
SiG-DMA^{V}	a	1.72	1.79	-
	b	1.71	1.84	1.84
	c	1.71	1.74	-
SiG-DMMTA^{V}	a	1.74	1.80	1.83
	b	2.27	2.22	1.67

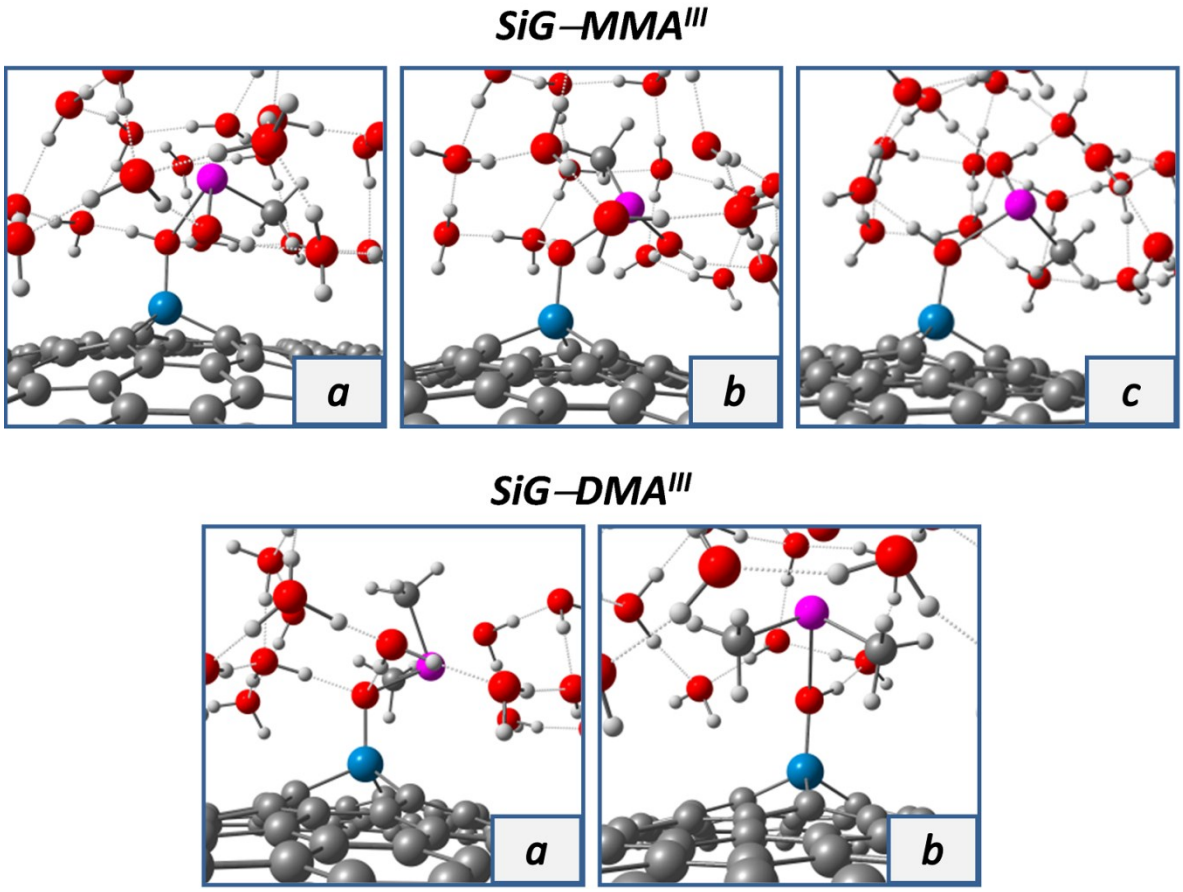

Fig. S1 Minimum energy conformations of MMA^{III} and DMA^{III} adsorbed onto SiG in a solvent environment; the pollutants are surrounded by 15 H_2O molecules with pointed hydrogen bonds.

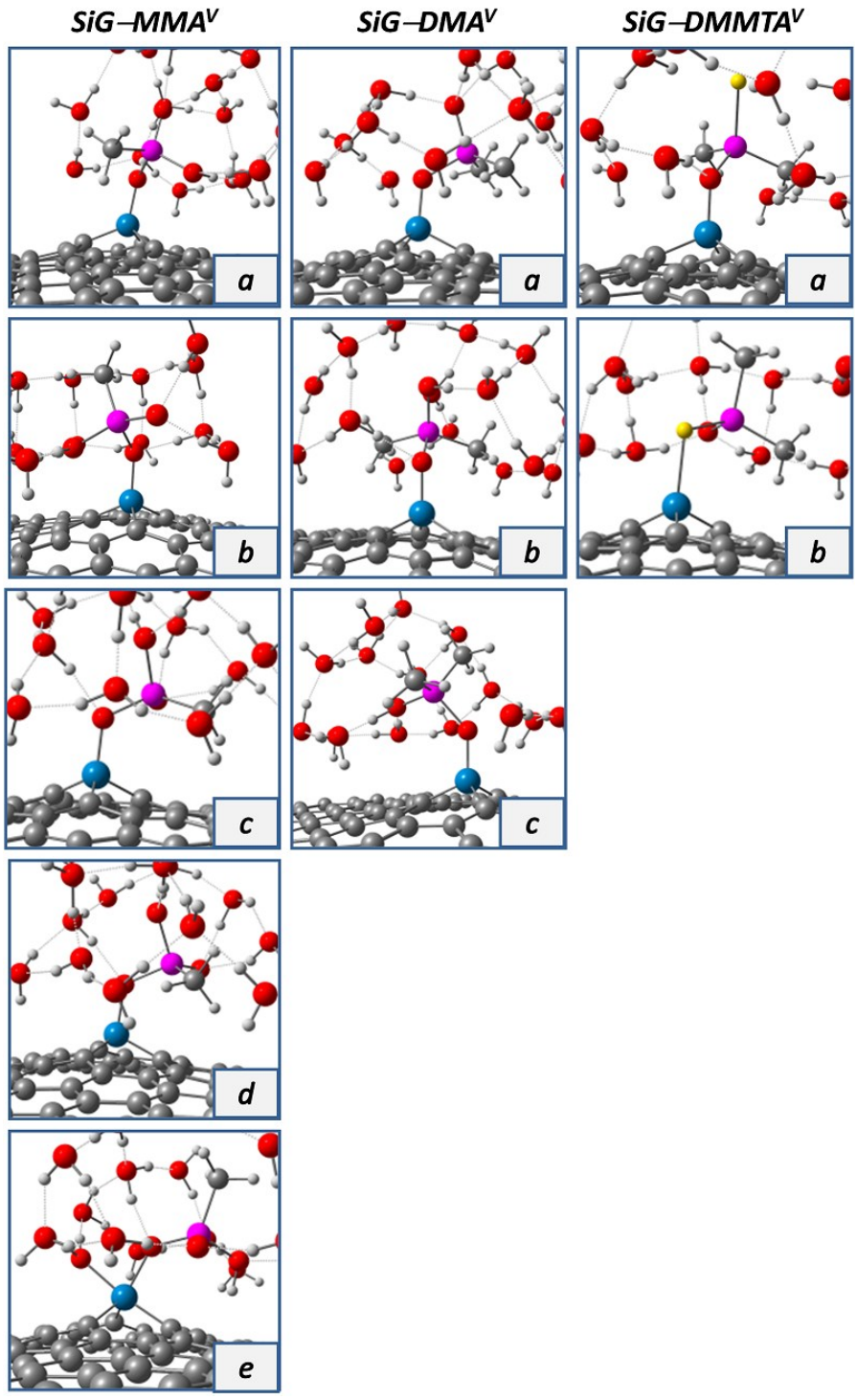

Fig. S2 Minimum energy conformations of MMA^V, DMA^V and $DMMTA^V$ adsorbed onto SiG in a solvent environment; the pollutants are surrounded by 15 H_2O molecules with pointed hydrogen bonds.