Supplemental Information

SI 1. Chemical structure and the DFT energies of fragments.

Fragment Name	Input Chemical Structure Optimized Geometry	UB3LYP/6-31G(d,p) Energy (eV)
Polyethylene Mechano-radical		-12852.8
Polyethylene Mechano-anion		-12851.7
Polyethylene Mechano-cation		-12846.2
Polyethylene Protonated Mechano-anion		-12871.1

Polyethylene Hydroxylated Mechano-cation		-14917.6
Polytetrafluoroethylene Mechano-radical		-80358.8
Polytetrafluoroethylene Mechano-anion		-80360.0
Polytetrafluoroethylene Mechano-cation	$\begin{array}{c} \textcircled{\textcircled{\begin{tabular}{c} & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & $	-80349.8

Polytetrafluoroethylene Protonated Mechano-anion	-80377.0
Polytetrafluoroethylene Hydroxylated Mechano-cation	-82424.2
Polydimethylsiloxane Si-terminated Mechano-radical	-35336.3
Polydimethylsiloxane O-terminated Mechano-anion	-37386.8

Polydimethylsiloxane Si-terminated Mechano-cation		-35330.7
Polydimethylsiloxane Protonated Mechano-anion same as Hydroxylated Mechano-cation	, I, O, I, O, I, OH Si O, Si OH	-37402.6

SI 2. Chemical Structure and DFT energies of water clusters and ions.

Water Chemical Structure	Optimized Geometry	UB3LYP/6-31G(d,p) Energy (eV)
[H ₂ O] ₁	.	-2079.5
H+	۲	0
ОН-	••	-2060.6

[H ₂ O] ₃	600 600 600 600	-6239.3
[H ₂ O] ₂ H ⁺	ی و	-4168.6
[H ₂ O] ₂ OH ⁻		-6223.0
[H ₂ O] ₅		-10399.8
[H ₂ O] ₄ H ⁺	<u>م</u> م	-8329.7
[H ₂ O] ₄ OH ⁻		-10384.3

[H ₂ O] ⁺	-10390.7
[H ₂ O] ₅	-10397.7