

Supplementary information for:

Robust surface coating materials for chemical warfare agent simulant detoxification using ladder-like poly(silsesquioxane) and metal–organic framework composites

Seungjae Lee,^{†a,b} Seungjae Hur,^{†a,c} Keunhong Jeong,^d Hoesun Hwang,^a Jungkyu Choi,^c Nithima Khaorapapong,^e Kyung-Youl Baek,^{‡a} Jin Young Seo,^{a,f,*} Yusuke Yamauchi,^{g,h} and Jongbeom Na^{a,g,i,*}

^a *Materials Architecturing Research Center, Korea Institute of Science Technology, Seoul 02792, Republic of Korea*

^b *Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul 03722, Republic of Korea*

^c *Department of Chemical and Biological Engineering, Korea University, Seoul 02841, Republic of Korea*

^d *Department of Chemistry, Korea Military Academy, Seoul 01805, Republic of Korea*

^e *Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

^f *Research Center for Bio-Based Chemistry, Korea Research Institute of Chemical Technology, Ulsan 44429, Republic of Korea*

^g *Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland, Brisbane, Queensland 4072, Australia*

^h *Department of Materials Process Engineering, Graduate School of Engineering, Nagoya University, Nagoya 464–8603, Japan*

ⁱ *KHU-KIST Department of Converging Science and Technology, Kyung Hee University, Seoul 02447, Republic of Korea*

[†] *Seungjae Lee and Seungjae Hur contributed equally to this work*

[‡] *Deceased, 10.03. 2023*

Corresponding Author E-mail: jyseo@krikt.re.kr (J. Y. Seo) and jongbeom@kist.re.kr (J. Na)

Keywords : Ladder-like Poly(silsesquioxane), Surface coating, Metal-organic Framework (MOF), Polymer Composites, Chemical Warfare Agents (CWA)

Table S1. Detailed amounts for synthesis of LCEISQs with different BPEI fraction.

Entry	Sample	30wt% BPEI in CHCl ₃ (g)	25wt% LPCPSQ in CHCl ₃ (g)
1	LCEISQ10	0.13	1.56
2	LCEISQ20	0.24	1.43
3	LCEISQ30	0.33	1.32
4	LCEISQ40	0.40	1.03
5	LCEISQ50	0.50	0.85

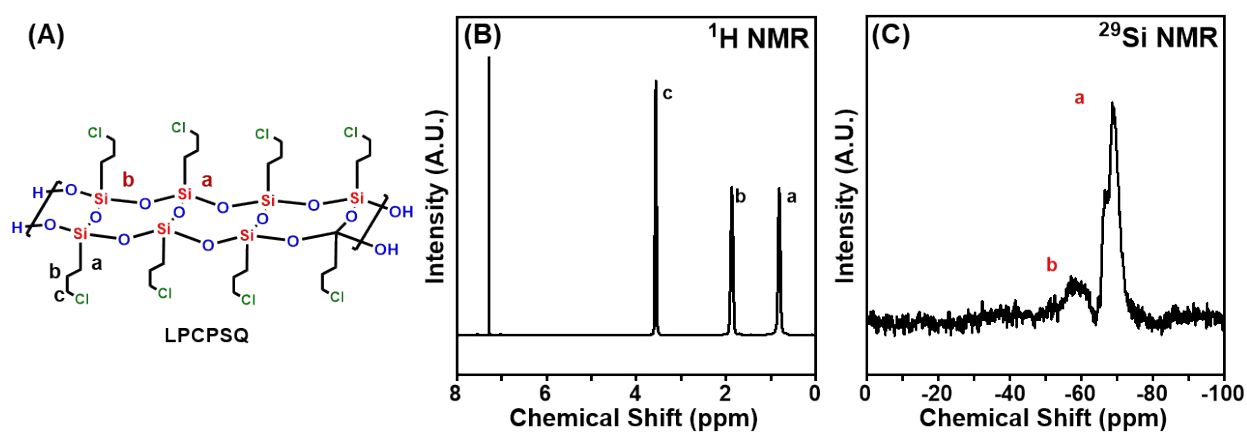


Fig. S1. (A) Chemical structure, (B) ¹H NMR spectrum, and (C) ²⁹Si NMR spectrum of synthesized LPCPSQ.

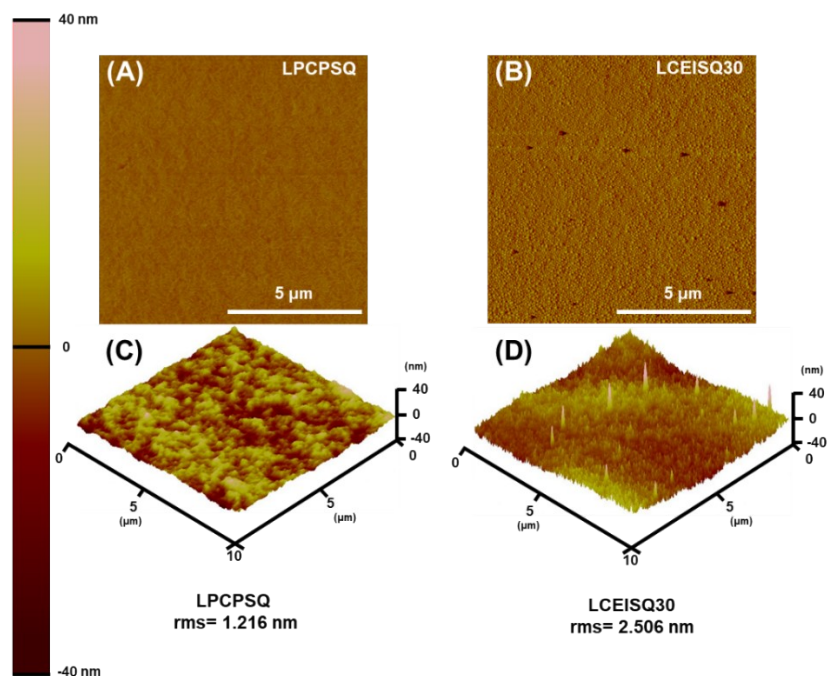


Fig. S2. AFM phase images and 3D topology of the (A, C) LPCPSQ and (B, D) LCEISQ30.

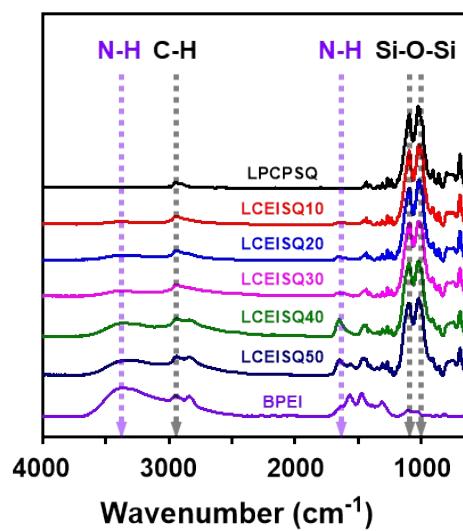


Fig. S3. FT-IR spectra of LCEISQs with varying BPEI contents.

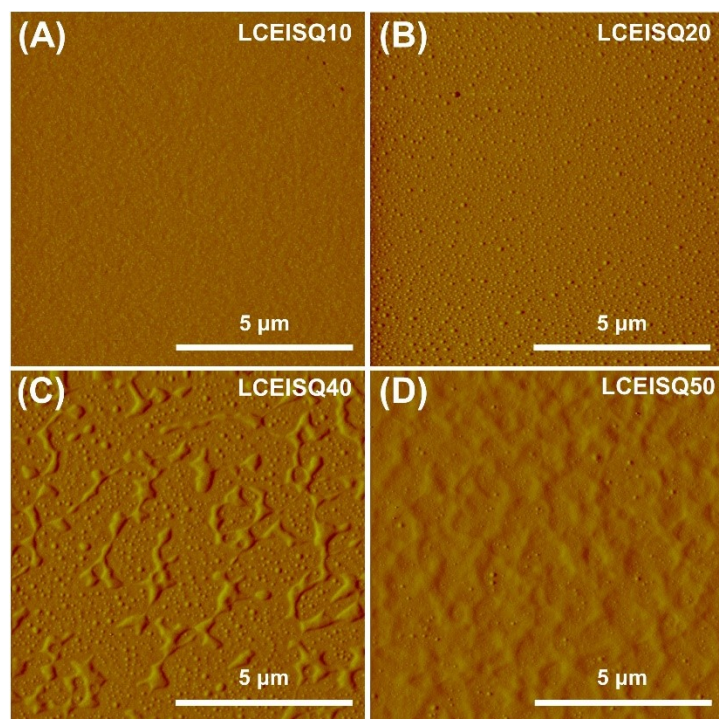


Fig. S4. AFM phase images of LCEISQs with various BPEI fractions (A) LCEISQ10, (B) LCEISQ20, (C) LCEISQ40, and (D) LCEISQ50.

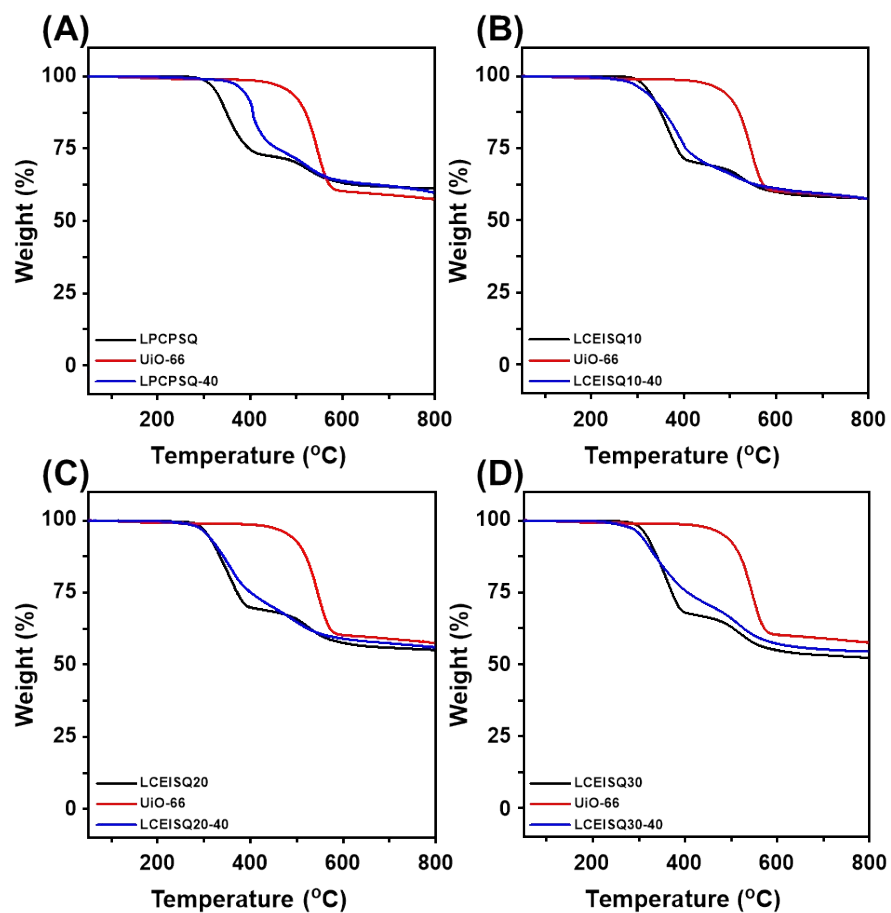


Fig. S5. TGA spectra of LCEISQ & UiO-66 composites, UiO-66, and LCEISQ with various composition (A) LPCPSQ-40, (B) LCEISQ10-40, (C) LCEISQ20-40, and (D) LCEISQ30-40.

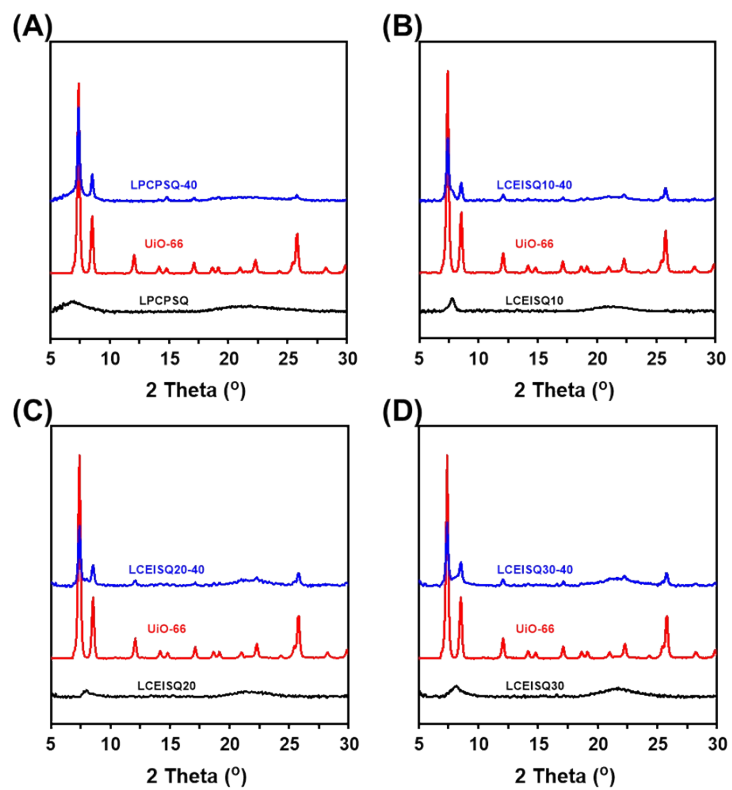


Fig. S6. XRD spectra of LCEISQ & UiO-66 composites, UiO-66, and LCEISQ (A) LPCPSQ-40, (B) LCEISQ10-40, (C) LCEISQ20-40, and (D) LCEISQ30-40.

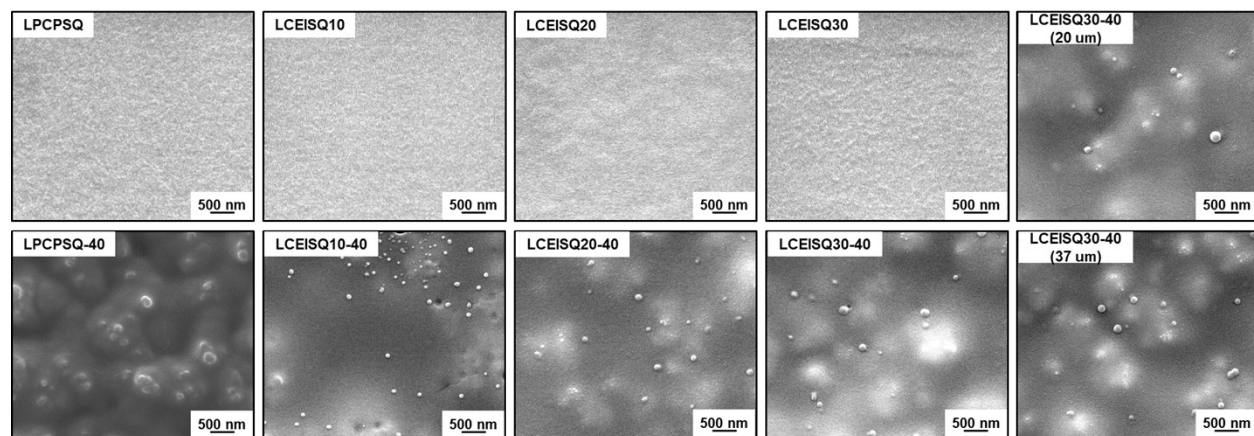


Fig. S7. SEM images of LPCPSQ, LCEISQs, and UiO-66 introduced composite films.

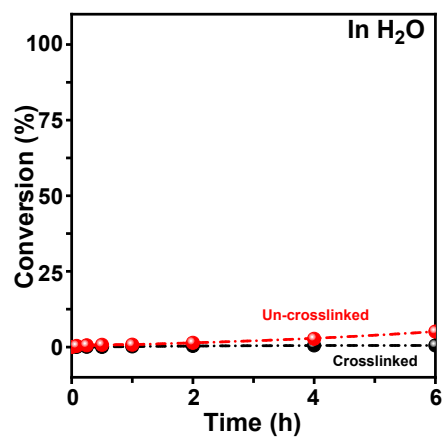


Fig. S8. MPO hydrolysis kinetics in a neutral solution of crosslinked and un-crosslinked LCEISQs.

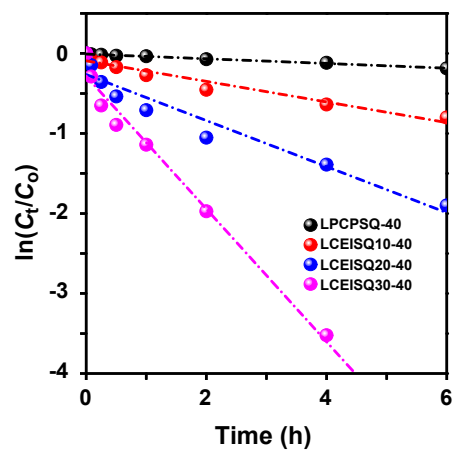


Fig. S9. MPO hydrolysis kinetics in a neutral solution ($\ln(C_t/C_0)$ vs. time plots) of UiO-66 introduced LCEISQs.

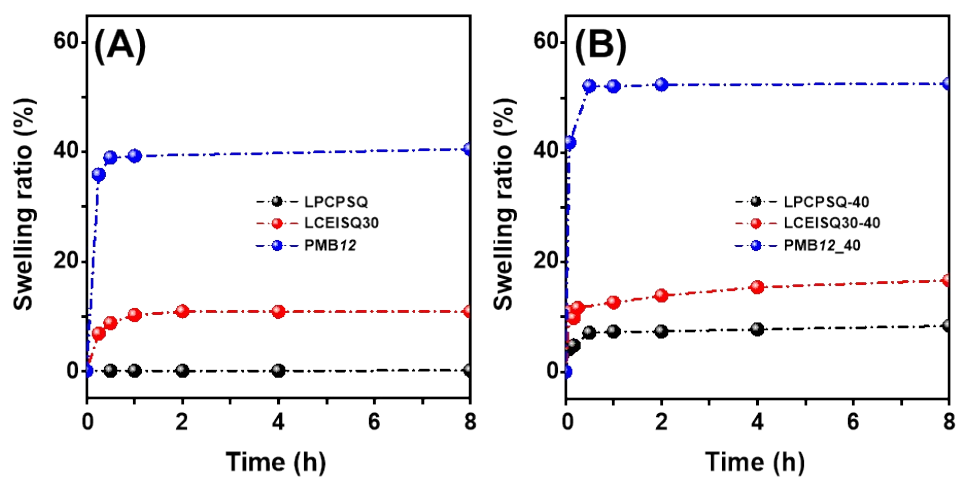


Fig. S10. Swelling test of (A) PMB12, LCEISQs, (B) UiO-66 introduced the composite film with PMB12, LCEISQs under aqueous solution.

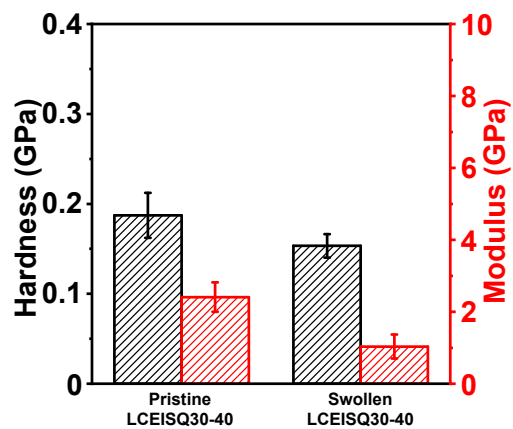


Fig. S11. Mechanical strengths (surface hardness and modulus) of pristine and swollen LCEISQ30-40.

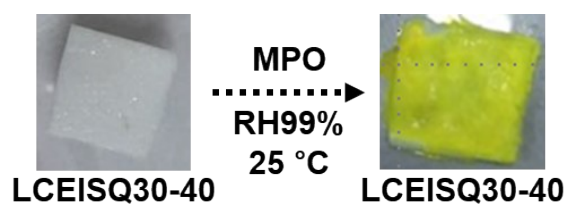


Fig. S12. Digital images of LCEISQ30-40 before and after MPO degradation under relative humidity conditions.

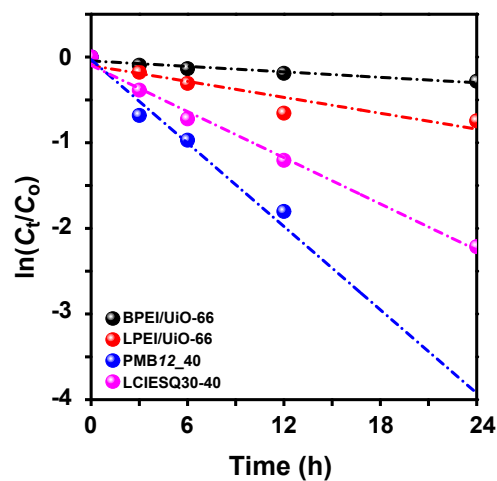


Fig. S13. MPO hydrolysis kinetics in the gas phase ($\ln(C_t/C_0)$ vs. time plot) of UiO-66 introduced LCEISQs

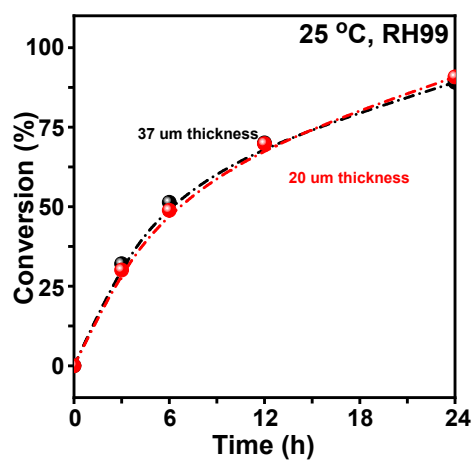


Fig. S14. MPO hydrolysis kinetics in the gas phase of LCEISQ30-40 with 20 and 37 μm thickness (same weight).