Supporting Information

Investigation on the Interface Structure and Filler Network Formation of Liquid Silicone Rubber/Silica Nanocomposites Based on ATR-FTIR Spectroscopy and Chemometrics \*\*

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Fig.S1. FTIR spectra results after normalization of bound rubber extracted after (a)0 days; (b)7 days; (c)14 days; (d)21days, respectively.



Fig.S2. particle size distribution with (a)different silica loadings; (b)bound rubber in different days after extraction of toluene



Fig.S3. TGA curves were obtained under nitrogen atmosphere from 40 °C to 800 °C



**Fig.S4.** loading spectrum of PCA of silicon rubber/silica nanocomposites with (a-c) combination; (d-f)30phr; (g-i)35phr; (j-l)40phr; (m-o)45phr; (p-r)50phr, respectively.



Fig.S5. 2D PCA score plots of silicon rubber/silica nanocomposites with (a-c) combination; (d-f)30phr; (g-i)35phr; (j-l)40phr; (m-o)45phr; (p-r)50phr, respectively.

Table S1. Software environment used for the chemometrics				
Name	Description	Version		
spyder	The scientific python development environment.	4.1.4		
scikit-learn	A set of python modules for machine learning and data mining.	0.23.1		
pandas	High-performance, easy-to-use data structures and data analysis	1.0.5		

	tools.	
matplotlib	Publication quality figures in python.	3.2.2
numpy	Array processing for numbers, strings, records, and objects.	1.18.5
	Table S2. Hyperparameter used in KMeans clustering	
Name	Description	Value
Initialization	Ensure centroids initialization stability	k-means++

Max iterations	A set of python modules for machine learning and data	500		
mining.				
Tolerance	Define convergence criteria	1e-4		
Random state	Guarantee reproducibility	10		



Fig.S6. 2D PCA score plots of (a-c) silicon rubber/silica composites and bound rubber extracted for (d-f)7 days; (g-i)14 days and (j-l)21 days, respectively.



Fig.S7. 2D PCA loadings plots of (a) PC1 and PC2; (b)PC1 and PC3 and (c)PC2 and PC3, respectively.

To determine whether the differences in the principal component scores among the five groups of samples are significant, a one-way analysis of variance (ANOVA) is performed. The null hypothesis in one - way ANOVA is that the means of the principal component scores for all groups are equal. The F-statistic is calculated as the ratio of the between-group variance to the within-group variance. If the calculated F-value is large enough, it indicates that the between-group variance is much larger than the within-group variance, suggesting that there are significant differences among the groups. The p-value is then calculated based on the F-distribution with appropriate degrees of freedom. If the p-value is less than the chosen significance level (usually 0.05), the null hypothesis is rejected, and it is concluded that there are significant differences among the groups. In this case, as shown in Table S1, for PC2 and PC3, the p-values are less than 0.05, so it can conclude that there are significant differences among the samples of different phr fillers for these two principal components. For Principal Component 1, the p-value is greater than 0.05, indicating no significant differences among the groups.

Table S3. Significance Test Results of Principal Components for Samples						
Principle Components	F-statistic	p-value	Significance Difference Judgment			
PC1	0.64	0.63	No			
PC2	11.51	2.07*10-8	Yes			
PC3	3.28	0.01	Yes			