Supporting Information

Research on the Influence of Cation–π Interactions Formed by Different Metal Cations on the Mechanical Properties of Epoxy Resin

Heshuang Li[#], Sijie Yin[#], Jingya Liu*, Qiaolin Tang, Qiang Peng, Ai Lu,Yunbo Xu***, JingJin Huang****, and Ming Kang[†]**

School of Material and Chemistry, State Key Laboratory of Environment-friendly Energy Materials, Southwest University of Science and Technology, Mianyang 621010, P.R. China

*Zigong Centre for Disease Control and Prevention, Institute of Physical and Chemical, Zigong 643000, P.R. China

**National Key Laboratory of Chemical Explosion Safety, Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang, 621900, China

***Sichuan Shutai Chemical Technology Co., Ltd, Suining 629399, P.R. China

****Sichuan Coremer Materials Co., Ltd., Mianyang 621010, P.R. China

Keywords: cations-π interaction, epoxy resin, mechanical properties, weak interaction.

* Corresponding authors.

E-mail addresses: dyw510@126.com (Ming Kang),

[1] These authors contributed equally to this manuscript.

1. Characterization

Fourier Transform Infrared Spectroscopy (FTIR spectroscopy)： FTIR spectra were measured on a Nicolet 380 FTIR spectrometer equipped with a deuterated triglycine sulfate (DTGS) detector and a Ge/KBr beam splitter using the KBr pellet technique. Each sample of 2.0 mg was mixed with 200 mg of KBr in an agate mortar to form pellets during the test.

Fluorescent Emission Spectroscopy: Fluorescent emission spectroscopy was collected on a Shimadzu RF-6000 fluorescence spectrometer with excitation wavelength of 365 nm and excitation slits of 5 nm. The wavelength scanning range is 400-600 nm.

Ultraviolet/visible Light (UV/vis) Absorption Spectroscopy: UV-Visible spectroscopy was performed on a ShimadzuUV-2600 instrument. The wavelength scanning range is 200-300 nm. Solid UV/vis absorption spectroscopy were measured by placing a polymer coated quartz sheet in the passageway of incident light using quartz sheet as the background.

The stress-strain experiments: The stress-strain experiments were carried out on a universal testing machine (WDW-100, Changchun research institute of testing machines, Jilin, China) at room temperature. Testing speed for all samples was 2 mm min^{-1}.

The thermogravimetric analysis (TGA): TGA was performed on a Mettler Toledo TGA/SDTA851e over a temperature range of 25-700 °C at a heating rate of 10 °C min^{-1} under a nitrogen atmosphere.

Differential Scanning Calorimetry (DSC): DSC measurements were carried out on a TA Instruments Q2000 calorimeter. Samples were sealed into a standard aluminum pan. The scan was carried out in nitrogen atmosphere at a flow rate of 200 mL min^{-1} over a temperature range of 20-300 °C at a scanning rate of 10 °C min^{-1}. DSC measurements are conducted with two warm-up cycles to mitigate potential thermal history interferences.

Field-Emission Scanning Electron Microscope (FE-SEM): The cross-sectional scanning of the experimental sample was performed on a field emission scanning electron microscope Ultra55 (Zeiss, Germany).

Dynamic mechanical analyzer(RSA-G2): DMA and stress relaxation tests were conducted on this instrumention (TA).The DMA test conditions were a temperature increase rate of 3%℃/min from 30℃ to 150℃.A stress relaxation experiment was performed for 10 minutes at a strain of 2% and 90℃.

VTMR-20-010V-I Low-Field Nuclear Magnetic Resonance Analyzer: Using 5000KHz sampling bandwidth, 256 accumulations, and CPMG-VD sequence for testing (Niumag Company).

2. Theoretical calculation methodologies based on quantum chemistry and atom molecular dynamics.

Figure S1, S2 show the theoretical calculation data of X^{n+}($X=Na^{+}$ and K^{+}).Every **a** and **b** display the

isosurface plots (IRI) and scatter plots of IRI versus sign(λ_2)ρ after optimizing the designed X^{n+}-π interaction using the QC (DFT) method, revealing the weak interaction between Na^+ and indoles (Na^+-π interaction). Every **c** shows the variation of cation–π interaction strength with the distance between X^{n+} and indole groups. Every **d** presents the molecular orbital energy gap of the cation–π interaction. Every **e** illustrates the radial distribution function (RDF) of the distance between X^{n+} and indole.

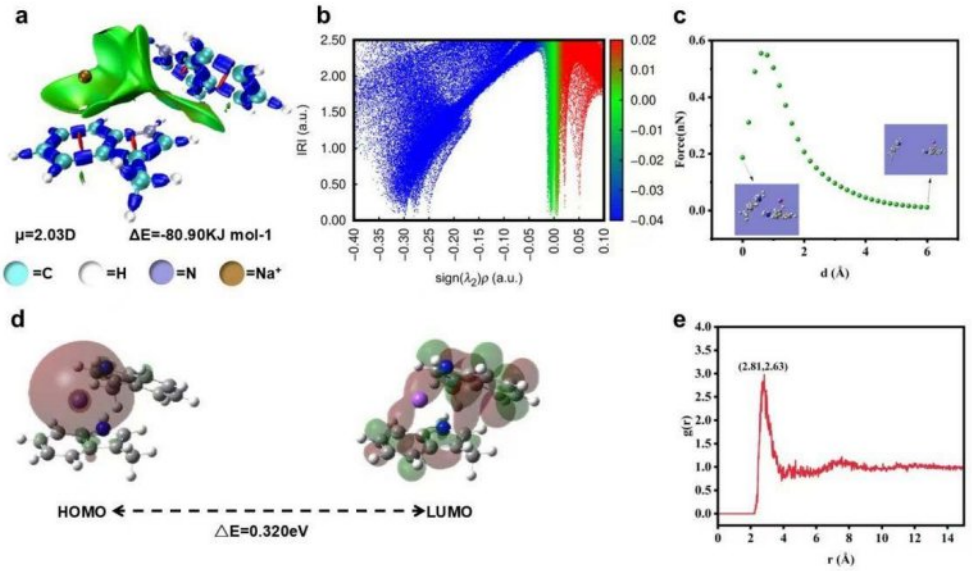

Figure S1 (a) IRI plot of Na^+ cation–π interaction; (b) IRI scatter plot; (c) variation in cation–π interaction strength with the distance between Na^+ and the indole group; (d) molecular orbital energy gap of the cation–π interaction; (e) radial distribution function (RDF) of the distance between Na^+ and indole.

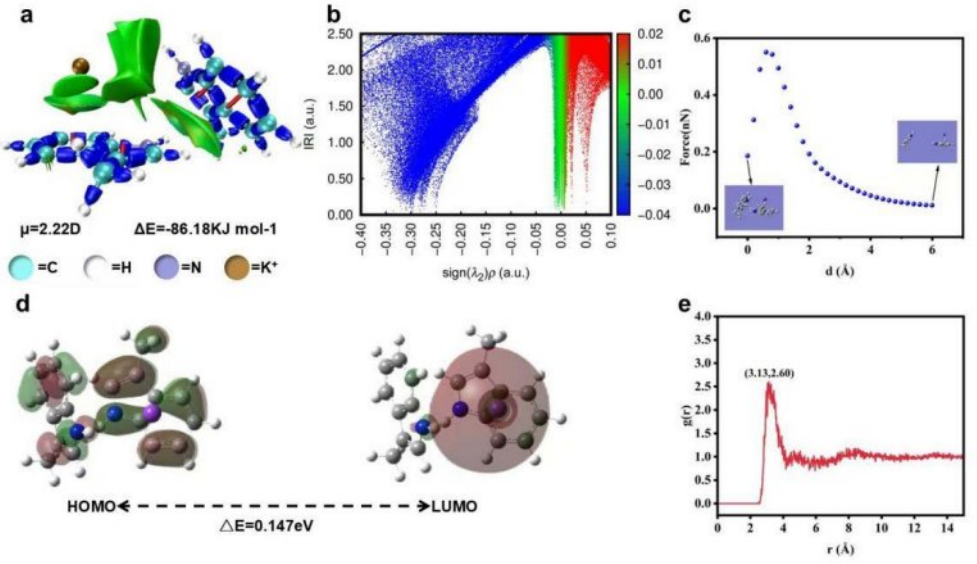

Figure S2 (a) IRI plot of K^+ cation–π interaction; (b) IRI scatter plot; (c) variation in cation–π interaction

strength with the distance between K^+ and indole group; (d) molecular orbital energy gap of cation–π interaction; (e) radial distribution function (RDF) of K^+-indole distance.

3. Statistical analysis of mechanical tensile tests。

All tensile data in the system are derived from five tests, excluding the maximum and minimum values. The remaining three test data are shown in the following **Table S1** and **S2.** Then, calculated the average and standard deviation based on these three tests, resulting in the error bars, as shown in the following **Figure S3**.

Table S1. Stress Data Sheet

Sample	Serial number(1 to 3) Stress(MPa)			Mean	Standard deviation	RSD(%)
	1	2	3			
CIEP-Na-5	50.01	46.65	48.01	48.22	1.69	3.50
CIEP-Na-10	51.30	51.22	46.72	49.74	2.62	5.26
CIEP-Na-15	45.71	45.63	45.52	45.62	0.09	0.21
CIEP-Na-20	55.00	58.45	54.02	55.81	2.33	4.18
CIEP-Na-25	51.90	51.74	52.77	52.13	0.55	1.06
CIEP-Mg-15	42.47	47.10	54.04	46.53	3.81	8.19
CIEP-Mg-20	53.18	51.49	60.51	55.06	4.79	8.70
CIEP-Mg-25	57.44	53.09	47.38	52.63	5.04	9.58
CIEP-Mg-30	60.23	62.88	58.47	60.52	2.21	3.66
CIEP-Mg-35	55.8	62.07	58.73	58.86	3.13	5.33
CIEP-K-5	53.71	53.56	50.45	52.57	1.84	3.50
CIEP-K-10	47.15	46.28	54.27	49.23	4.38	8.90
CIEP-K-15	55.26	54.18	52.00	53.81	1.66	3.08
CIEP-K-20	58.73	65.00	65.62	64.11	3.81	6.03
CIEP-K-25	51.43	48.87	48.06	49.43	1.78	3.60

Table S2. Strain Data Sheet

Sample	Serial number (1 to 3) Strain (%)			Mean	Standard deviation	RSD (%)
	1	2	3			
CIEP-Na-5	4.80	4.49	4.63	4.64	0.16	3.34
CIEP-Na-10	4.42	4.75	4.62	4.60	0.17	3.61
CIEP-Na-15	5.17	5.38	4.21	4.92	0.62	12.67
CIEP-Na-20	6.80	6.70	6.87	6.79	0.09	12.58
CIEP-Na-25	5.01	6.44	6.24	5.90	0.77	13.13
CIEP-Mg-15	6.76	7.11	6.13	6.67	0.50	7.44
CIEP-Mg-20	7.49	8.59	8.08	8.05	0.55	6.83
CIEP-Mg-25	10.01	10.14	12.39	10.85	1.34	12.33
CIEP-Mg-30	8.10	9.52	7.60	8.41	1.00	11.84
CIEP-Mg-35	6.38	7.17	7.39	6.98	0.53	7.60
CIEP-K-5	4.92	5.21	6.15	5.43	0.64	11.84
CIEP-K-10	5.26	6.02	5.23	5.50	0.45	8.13
CIEP-K-15	6.11	6.08	7.00	6.40	0.52	8.17
CIEP-K-20	7.39	6.87	6.13	6.80	0.63	9.31
CIEP-K-25	5.87	4.90	5.12	5.30	0.51	9.60

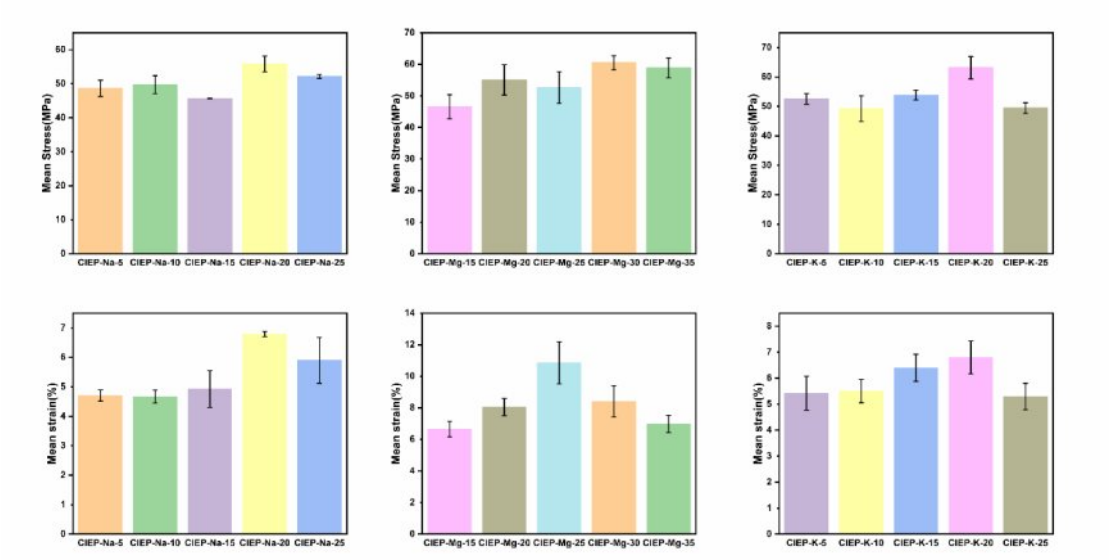

Figure S3. Error bars