Supporting Information

Efficient Neutron Radiation Shielding by Boron-Lithium Imidazolate Frameworks

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S1 Experimental Section

Synthesis of BIF1: Sodium tetrakis(imidazoly)borate (0.1830 g, 0.61 mmol) and $LiNO_3$ (0.2022 g, 2.9 mmol) in a mixed 2-amino-1-butanol (2 ml)/CH_3CN (8 ml) solution were placed in a 20 ml vial with ultrasonication for 30 min. The sample was heated at 85 ℃ for 3 days, and then cooled to room-temperature. After washed by acetone for three times, the colorless crystals were obtained. NaB(Im)4(Alfa-Aesar, 98%), $LiNO_3$ (Aladdin, 99%), 2-amino-1-butanol (TCI) and CH_3CN were used as received. AFG-90H epoxy, (Shanghai Huayi Resins Co., Ltd.) was selected as the epoxy monomer, with 4, 4' -diaminodiphenylsulfone (named as DDS, Shanghai Huayi Resins Co., Ltd.) as the curing agent.

Synthesis of Ep-complexes: To prepare AFG-90H epoxy resin (Ep)-based composites, varying amount of BIF1, $NaB(Im)_4$-$LiNO_3$, B_4C were added into the mixture of Ep component A and component B(mass ratio = 2:1), which was stirred for 10 min. The amount of Boron is 1% in all the samples except the pure Ep sample. 26.5% wt of BIF1 was added into the AFG-90H Ep and stirred for 10min. After degassing under vacuum, the mixture was poured into silicone molds and heated in setting processing (100 ℃ for 2 hours, 120 ℃ for 2 hours, 140 ℃ for 2 hours, 160 ℃ for 2 hours and 200 ℃ for 2 hours). The pure Ep sample were prepared following the same procedure as above, by eliminating the process of adding BIF1. The Ep-$NaB(Im)_4$-$LiNO_3$ and Ep-B_4C were prepared following the same procedure as above, added with 28% wt $NaB(Im)_4$, 0.6% wt $LiNO_3$ and 1.28% wt B_4C to instead of BIF1.

Characterization and Method: X-ray diffraction (XRD) was collected from 5° to 50° on a Bruker D8 advance diffractometer with Cu K_α radiation (λ = 1.54056 Å) with a Lynxeye one-dimensional detector. Fourier transform infrared (FT-IR) spectra were measured using Nicolet Nexus 470 with the KBr squashtechnique. Thermogravimetric analysis (TGA) were recorded on a NETZSCH STA449F3 instrument in the temperature range of 30 to 900 ℃ at a 10 ℃/min heating rate under nitrogen. Scanning electron microscopy (SEM, Phenom Pro, Phenom-world B.V.) was performed on the fracture surface of Ep-BIF1 composites with 15 keV electron beam. An Agilent 7700 ICP-MS equipped with a GeoLasPro 193 nm ArF excimer laser was used for the multi-element analyses. All recording parameters of LA-ICP-MS were optimized for both the reference materials and the samples. The scans were made in as identical location as possible. To prove the structural stability of BIF1 and Ep-BIF1 under high energy radiation, the samples were conducted under 50, 100, and 200 kGy using a ^{60}Co irradiation source (60,000 Curie) with a dose rate of 1.2 kGy / hour.

Neutron shielding experiment: The Am-Be neutron and thermal neutron shielding capability of composite materials were measured using an experimental setup in Nanjing University of Aeronautics and Astronautics.[1] A cadmium sheet with a thickness of 1 mm was selected as thermal neutrons absorber. Neutron shielding rate was calculated by the following equation:

$$R_{tot} = \frac{N_0 - N_{sample}}{N_0}$$

where R_{tot} represents the neutron shielding rate; N_{sample} represents the count rate of neutron detector with the sample; N_0 represents the count rate of neutron detector without the sample.

The shielding rate for thermal neutron was calculated by the following equation:

$$R_{thermal} = \frac{(N_0 - N_{sample}) - (N_{0Cd} - N_{sampleCd})}{N_0 - N_{0Cd}}$$

Where $(N_0 - N_{sample})$ is the total reduced count after adding sample; $(N_{0Cd} - N_{sampleCd})$ is the count except thermal neutrons contribution; $(N_0 - N_{0Cd})$ is the count of thermal neutron contribution.

S2 Supplementary Data

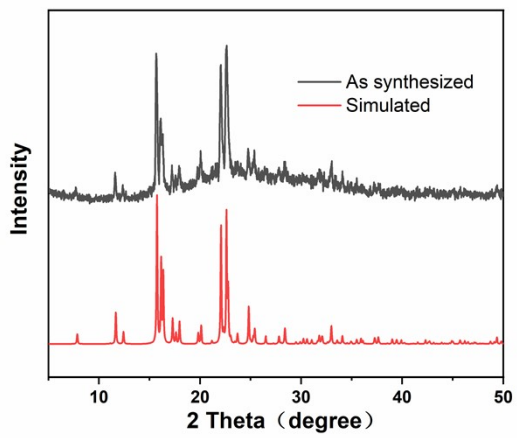

Figure S2.1. The PXRD patterns of BIF1 as synthesized and the simulated one.

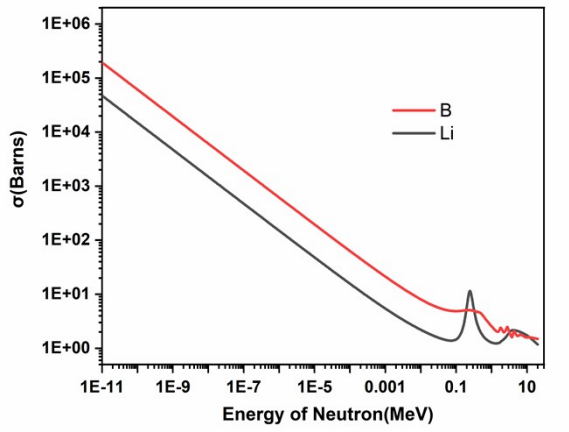

Fig S2.2. Neutron absorption cross section of boron and lithium.

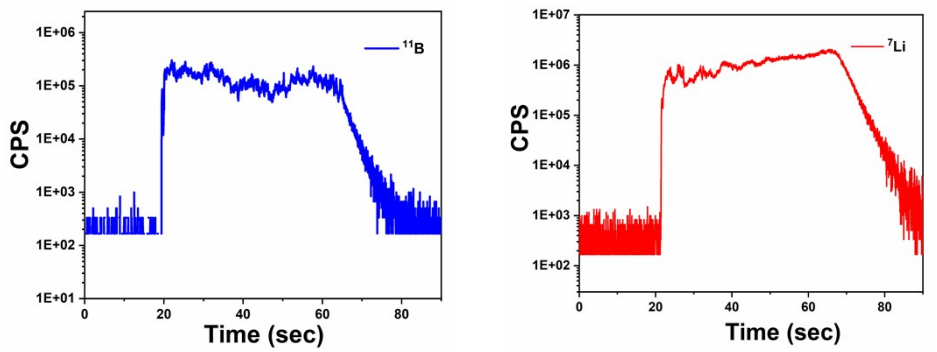

Figure S2.3. The time resolved analytical signals of ^{11}B(left)/ ^{7}Li(right) by LA-ICP-MS for Ep-BIF1.

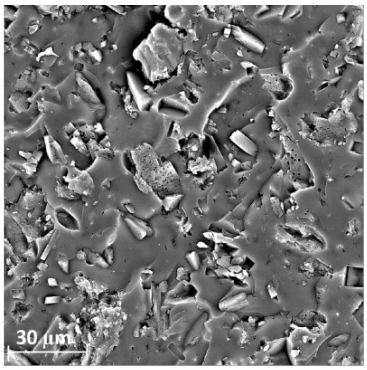

Figure S2.4. The SEM image of Ep-BIF1.

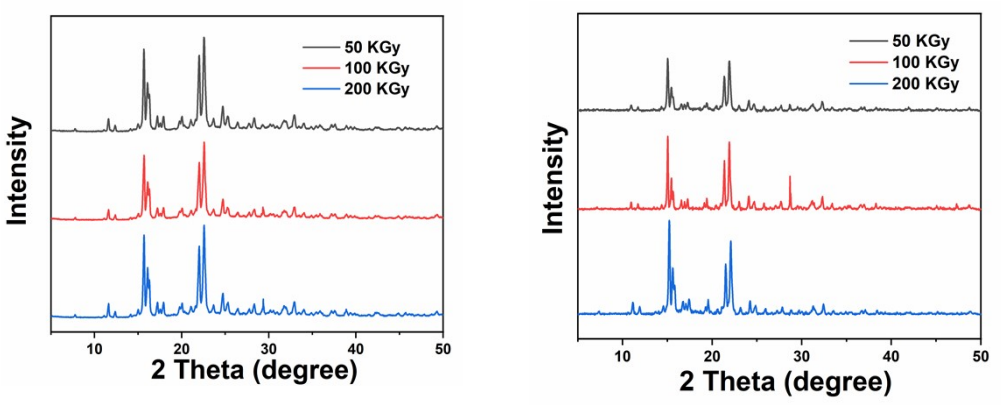

Figure S2.5. The PXRD patterns of BIF1 (left)and Ep-BIF1 (right) after exposure under Co-60 γ radiation with various doses.

Figure S2.6. The demonstration of polymer complexes (from left to right, Ep, Ep-B_4C, Ep-BIF1, Ep-$NaB(Im)_4$-$LiNO_3$)

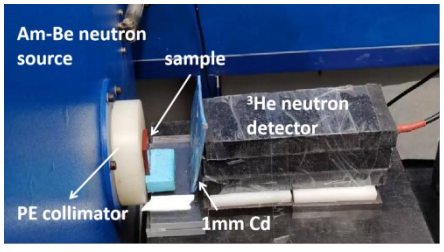

Figure S2.7. The view of Am-Be neutron source and instrument.

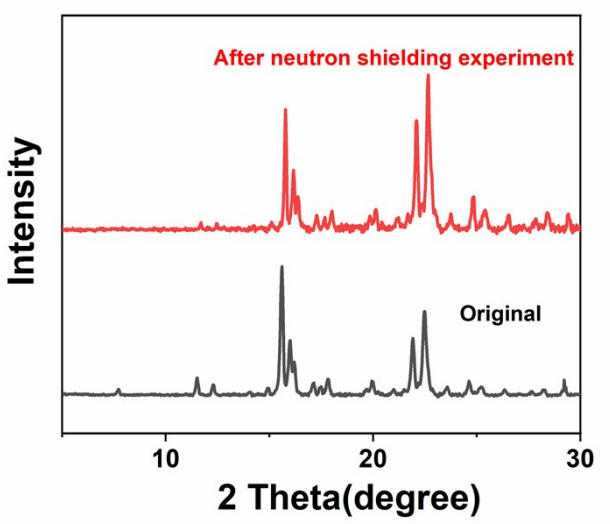

Figure S2.8. PXRD patterns of Ep-BIF1 before and after neutron shielding experiment.

Table S1. Test results for shielding rate of thermal neutrons and Am-Be neutron source.

	Shielding rate of thermal neutron (%)			Shielding rate of Am-Be neutron source (%)		
Thickness	0.5 cm	1 cm	1.5 cm	0.5 cm	1 cm	1.5 cm
Ep	40.5	53.33	64.2	29.55	37.99	45.97
Ep-B4C	49.31	65.67	73.18	31.86	44.09	51.47
Ep-BIF1	49.98	68.13	75.28	31.81	46.20	51.12
Ep-$NaB(Im)_4$-$LiNO_3$	49.80	67.05	73.45	31.89	45.22	49.99

Reference

1 D. Zhao, W. Jia, D. Hei, C. Cheng, J. Li, P. Cai, Y. Chen, *Radiation Physics and Chemistry*, 2022, **193**, 109954.