New approaches to self-healing, proper characterization methods for dynamic noncovalent bonds, and demonstration of simulations are introduced.

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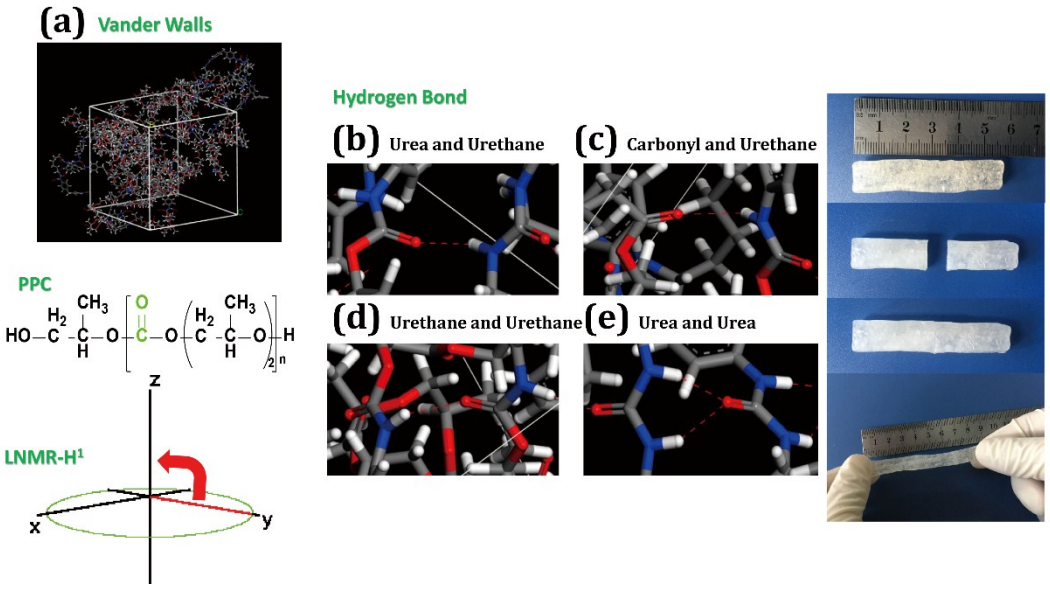

Supporting information

A self-healing elastomer based on an intrinsic non-covalent cross-linking mechanism

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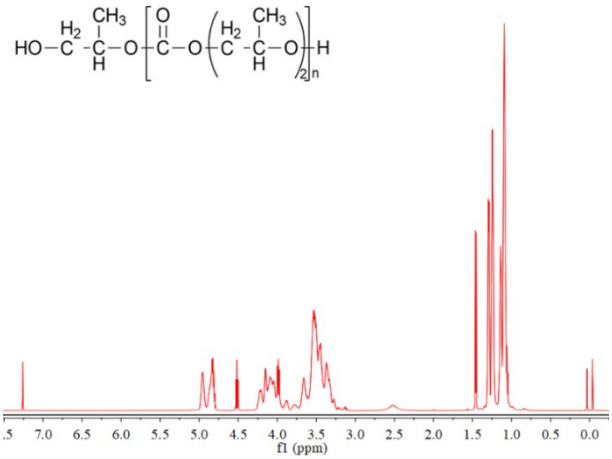
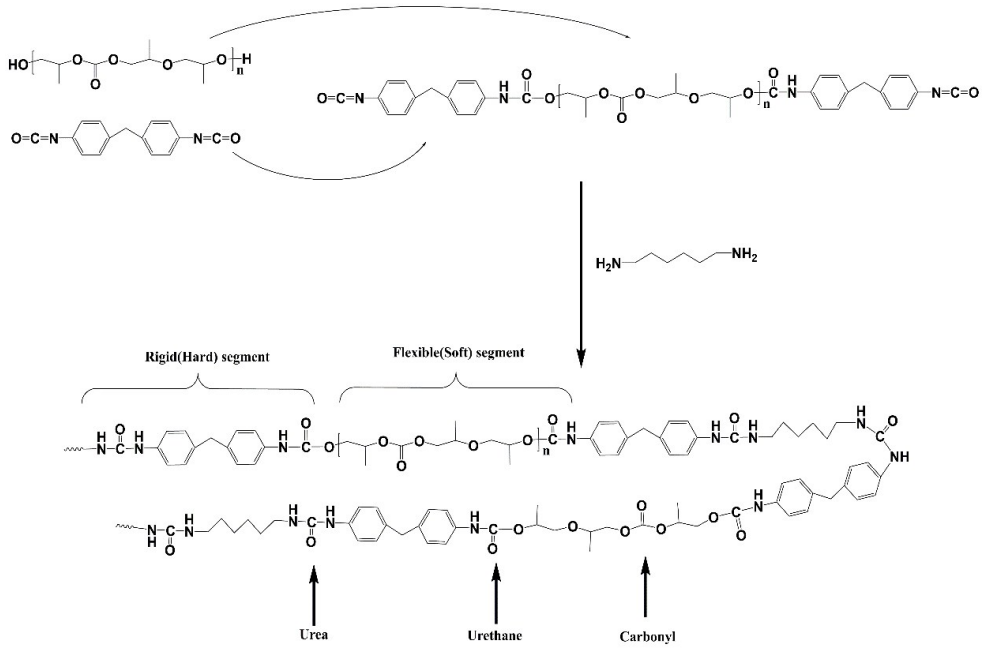
Information of the PPC: (Fig S1)

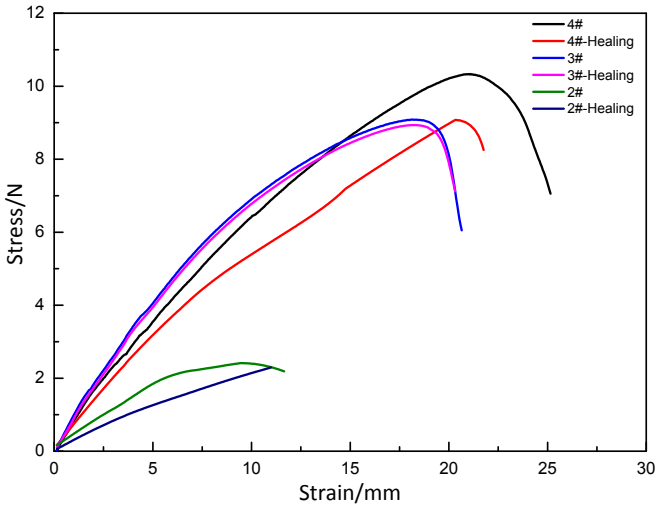
PPC-HNMR



Reaction process: (Fig S2)



The GPC of polypropylene carbonate polyurethane: (Fig S3)



The GPC of polypropylene carbonate polyurethane: (Fig S4)

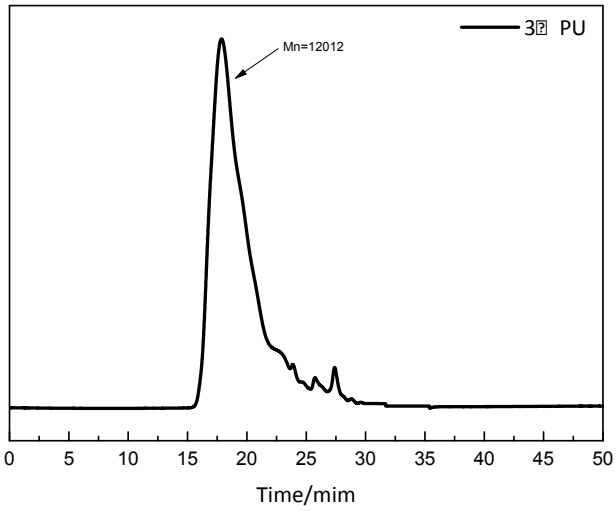
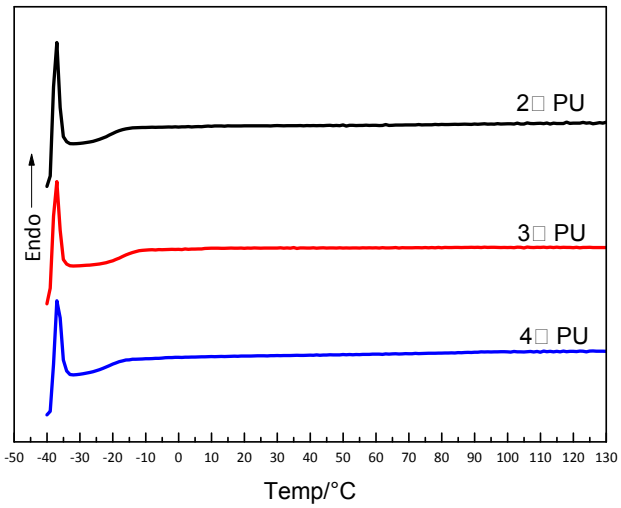


Table 1: Molecular weight and molecular weight distribution

Peak	Time/min	Mw	Mn
1	18.173	23306	12012
1	17.159	20290	12365

The DSC of polypropylene carbonate polyurethane: (Fig S5)



The XRD of polypropylene carbonate polyurethane: (Fig S6)

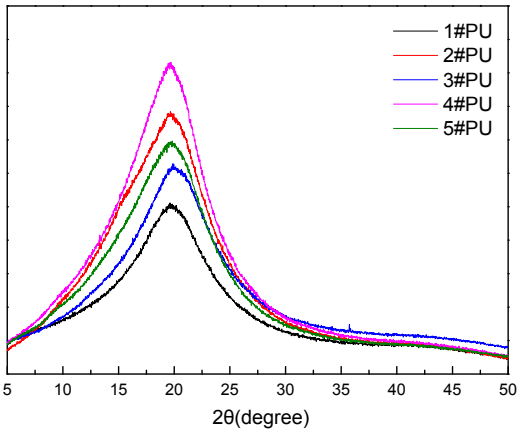
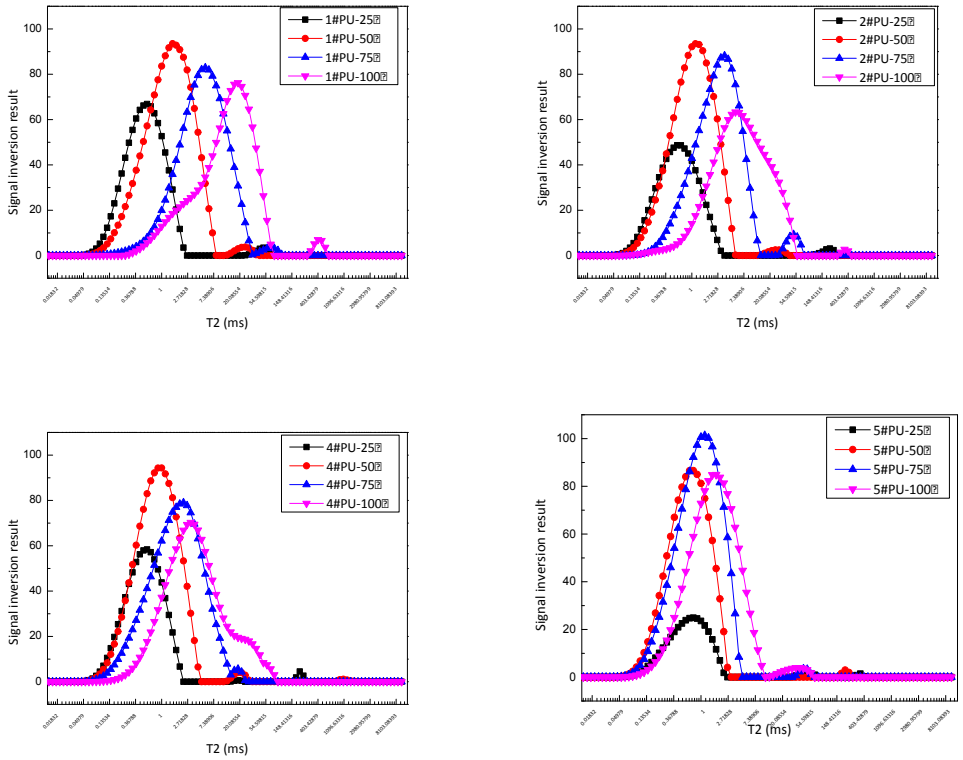


Table 2: Crystallinity and crystal size

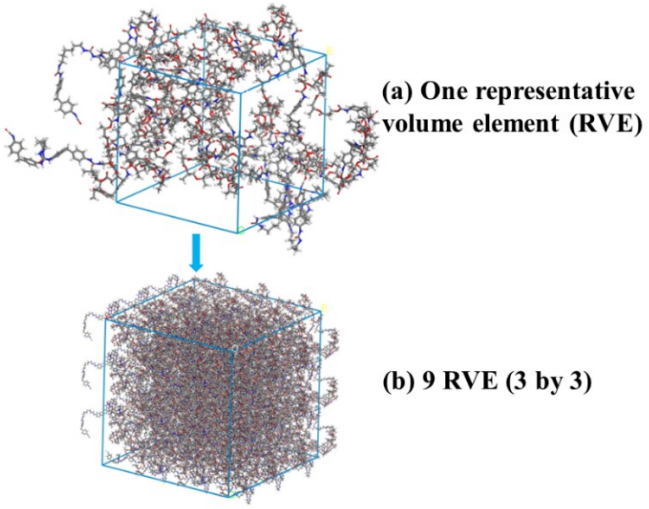
Serial number	1#PU	2#PU	3#PU	4#PU	5#PU
Half peak width	0.98	0.88	0.70	0.84	0.82
Zone size/nm	8.09	8.99	10.35	9.50	9.20
Crystallinity	0.05%	2.15%	2.99%	5.16%	6.68%

At 19.8 ° in the polymer material typical diffuse scattering peak, although able to compute certain crystallization in chengdu, but its low to DSC instrument can't detect, proof of no crystallization peak caused because of the aggregation of MDI. When the molecular weight of the material increases to a certain extent, MDI aggregation will definitely occur, and aromatic MDI aggregation will definitely cause crystallization of the material, thus affecting the healing performance of the material. Therefore, the molecular weight obtained in this paper is the optimal molecular weight for MDI type aromatic polyurethane to achieve healing.

LNMR of the hydrogen bonds of PPC-PU: (Fig S7)



Modeling and simulation details: (Fig S8)



The supercell with 9 representative volume elements (3 by 3)

The MD simulation software, Materials Studio, has an embedded Amorphous Cell Calculation tool which can build the 3D periodic cell expediently by packing the molecular chains randomly. The non-covalent encompassing Van der Waals, electrostatic and hydrogen bond interactions are described by force field, a series of equations describing interactions; that is, the non-covalent bonds are considered to create the 3D form as well as in the process of MD simulation.

The periodic boundary conditions can be observed by building the supercell with 9 representative volume elements (3 by 3), as shown in Fig. **S8**.

The kinds of the hydrogen bonds and length in PPC-PU: (Fig S9)

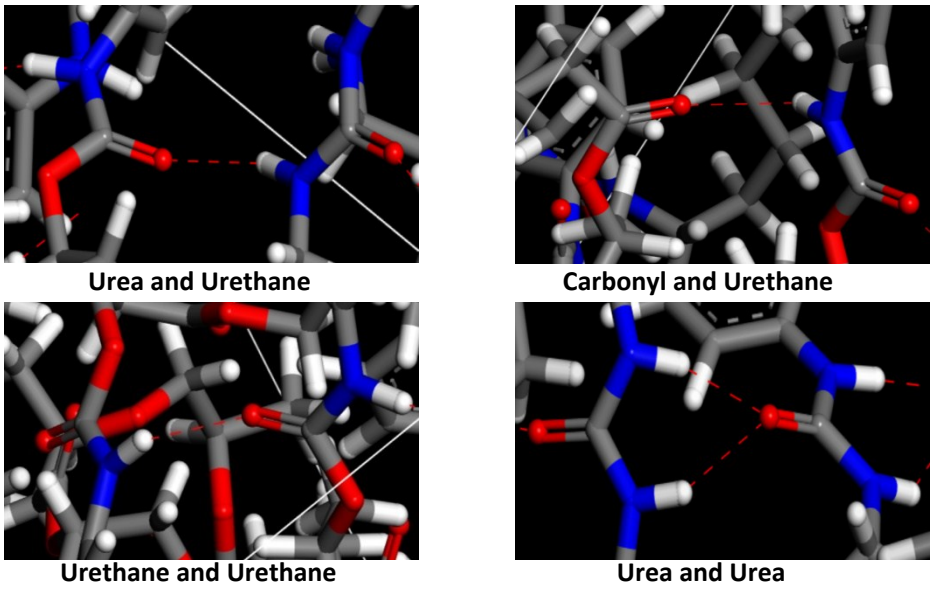
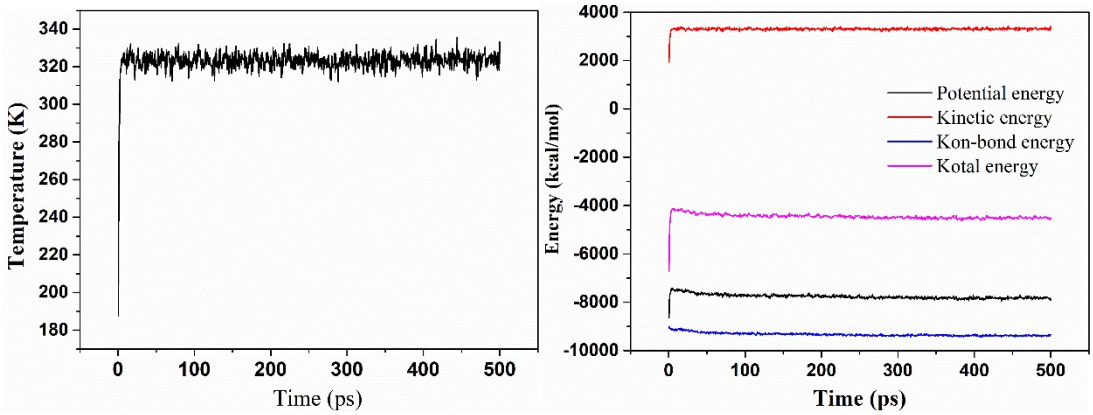


Table 3: Hydrogen bond length

Group	urea urethane	carbonyl urethane	urethane urethane	urea urea
Bond length	2.06594 Å	2.37951 Å	2.00062 Å	1.79747 Å

The relationship between healing time and healing performance of the PPC-PU: (Fig S10)



Temperature and energies evolution of 3#PU system at 50℃ after being subjected to 500 ps of NPT

In the simulation, the study on dynamic bonds exchange at each temperature is based on the equilibrium state of systems. After being subjected to 1 ns of NVT (constant number of particles, volume, and temperature) ensemble and 1 ns of NPT (constant number of particles, pressure, and temperature), the system reaches its equilibrium state based on the results of energies and temperature, as shown in Fig. S10. Therefore, we choose the temporal interval of 450-500 ps to analysis the hydrogen bonds exchange.