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Preparation and Interfacial Properties of Hydroxyl-Containing Polyimide Fibers

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Supplementary Files:

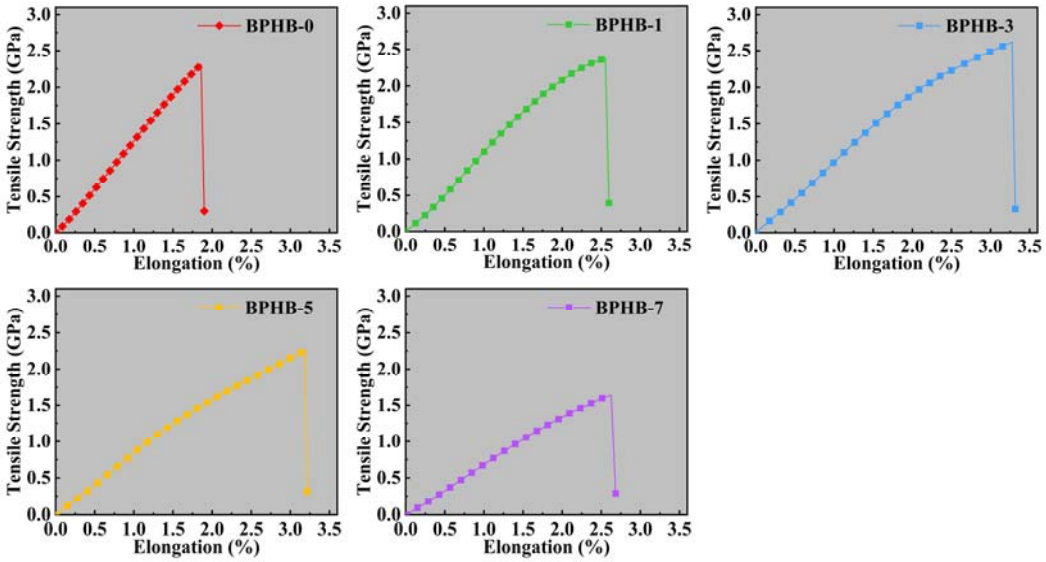

Figure S1. The typical tensile strength-elongation curves of the PI fibers with the various diamine molar ratios.

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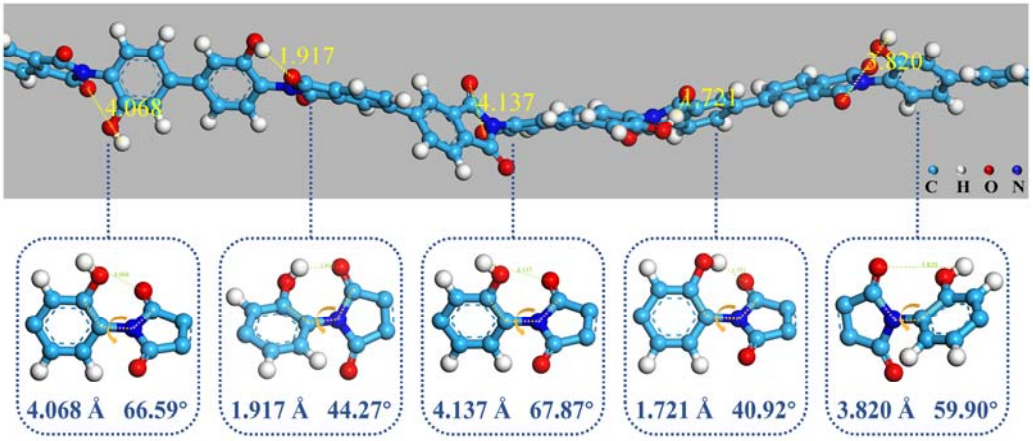

Figure S2. Simulated results of the dihedral angle between the imide ring and benzene ring containing -OH groups, as well as the atomic distance between the H atom of -OH and O atom of adjacent imide ring carbonyl for BPHB/HAB polymer chain in the lowest energy conformation.

The conformation of the BPDA/HAB polymer chain at the lowest energy is simulated using Materials Studio 8.0 software in Figure S2. Under the geometrically optimized conformation, the dihedral angles between the imide ring and benzene ring containing -OH groups are greater than 40°, implying that HAB moieties present a non-coplanar conformation with the backbones. In this situation, the probability of the distance between H atom of -OH and O atom of adjacent imide ring carbonyl being less than 2.6 Å is merely 40%. Generally, coplanar conformation along with atomic distance ($d_{(H...O)} < 2.6$ Å) are considered to be positive factors for the formation of intramolecular hydrogen bonds [39,44,45]. Consequently, the tendency to form intermolecular hydrogen bonds (-OH···O=C-) in BPHB fibers is simultaneously enhanced when more HAB monomer is introduced into BPDA/*p*-PDA/BIA molecular chains.

References [39,44,45] are cited in the main text.

Table S1. The surface elemental compositions of BPHB fibers with various diamine molar ratios.

PI Fibers	Element Content (%)			O/C
	C 1s	N 1s	O 1s	
BPHB-0	80.62	3.63	15.75	0.19
BPHB-1	80.22	3.51	16.27	0.20
BPHB-3	77.38	3.84	18.78	0.24
BPHB-5	75.95	3.95	20.10	0.26
BPHB-7	74.13	3.80	22.07	0.30