Supporting Information

Bio-based and recyclable adhesive based on β-hydroxyester bond and hydrogen bond via molecular dynamics simulation

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Table S1 The specific proportion of EMTO-VL

	Av mg·KOH/g	Hv mg • KOH/g	Ev mol/100g	EMTO-VL_2	EMTO-VL_4	EMTO-VL_6	EMTO-VL_8	EMTO-VL_{10}
EMTO/g	423.50	-	3.87	9.8	9.6	9.4	9.2	9
VL/g	146.91	359.04	-	0.2	0.4	0.6	0.8	1
Ratio(VL)/%	-	-	-	2	4	6	8	10

Av: Acid value, Hv : Hydroxyl value, Ev : Epoxy value.

Table S2 Detailed data of TGA tests of the EMTO-VL

	$T_{5\%}$[a]/°C	$T_{50\%}$[b]/°C	*Tmax*/°C	RC_{800}[c]/%	$T_{Oxidation}$ /°C
Lignin	201.2	> 800	296.1	51.80	277.6
V-Lignin	102.5	323.8	268.5	31.17	248.8
METO-VL2	103.1	384.9	445.8	5.91	--
METO-VL6	112.7	392.5	443.8	7.02	--
METO-VL10	124.7	400.6	442.5	9.64	--

a：The temperature at which the mass is lost by 5%.；b：The temperature at which the mass is lost by 50 %.；c: Amount of residual carbon at 800°C.

Table S3 Detailed data of molecular dynamics simulations on wood substrates

Substrate	Polymer	Number of chains	IAE(kcal mol^{-1})	Hydrogen bonds between layers
Wood	EMTO-VL	10	-335.08	12
Wood	MTO-VL	10	-213.99	0

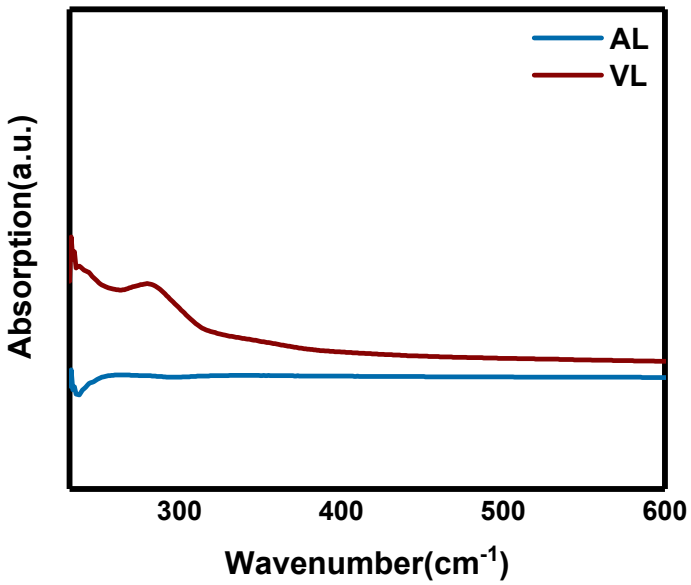

Fig.S1 Absorbance of AL, VL before and after dissolution measured by UV–vis–IR spectrophotometer

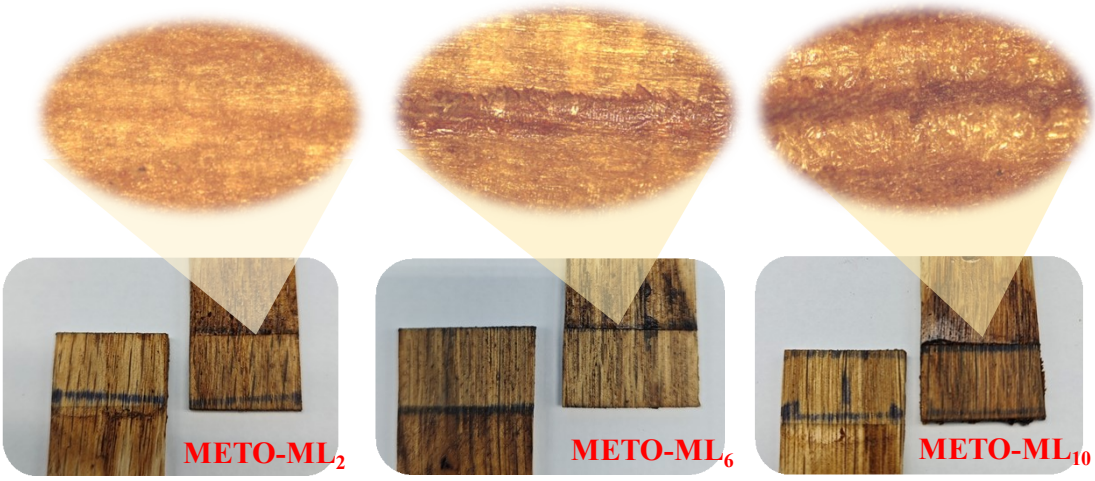

Fig.S2 The microscope images of EMTO-$VL_{2,6,10}$ after bonding wood chips

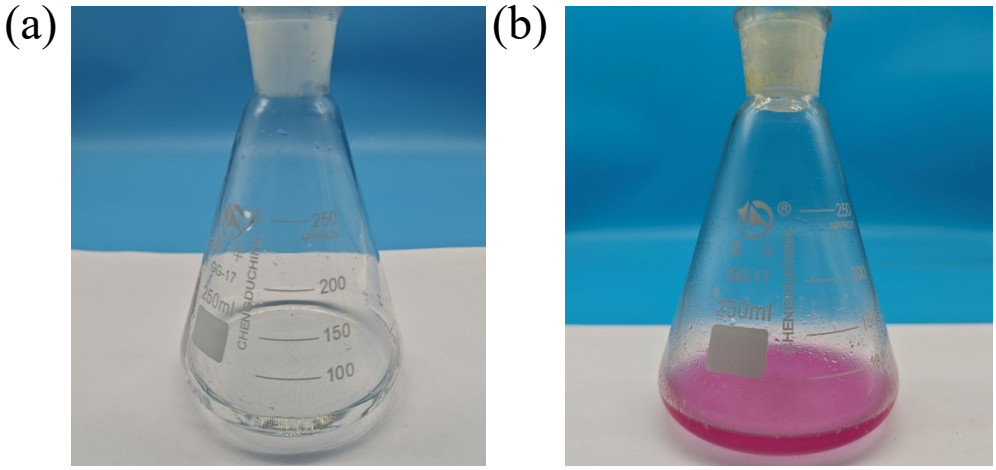

Fig. S3 Progressive diagram of titration.(a) Initial solution before titration.(b) The color of the solution reaches light pink and does not fade within 30s

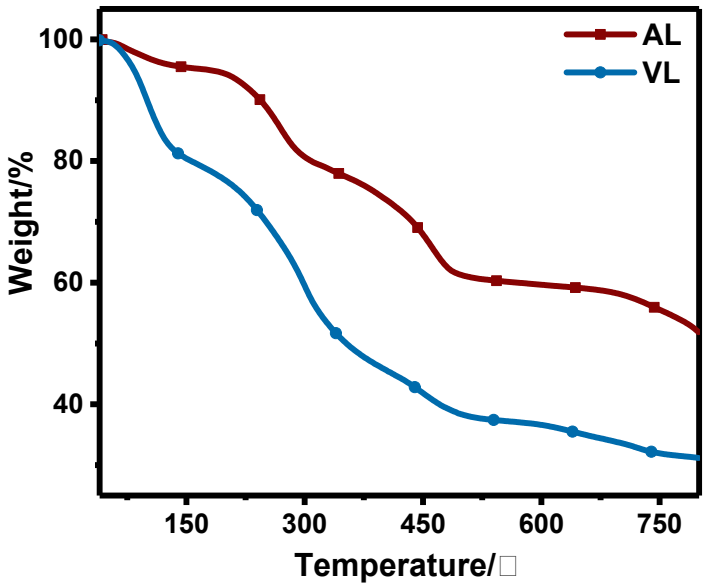

Fig.S4 TGA spectrum of lignin, vinyl- modified lignin in N_2.

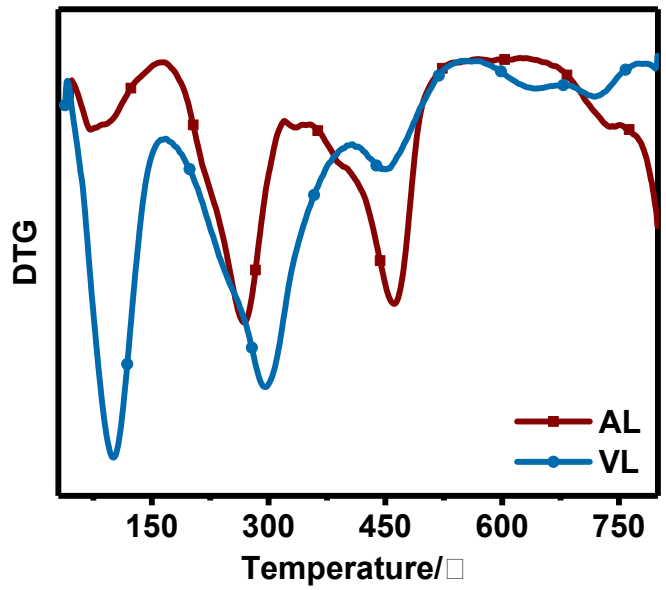

Fig.S5 DTG spectrum of lignin, vinyl- modified lignin in N_2

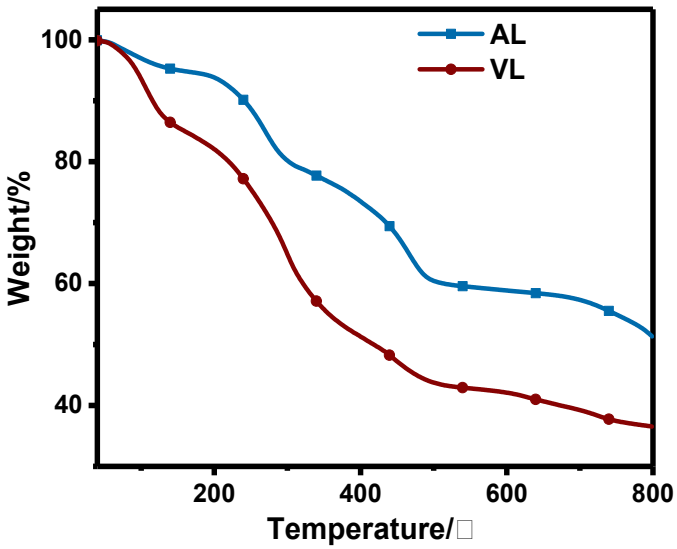

Fig.S6 TGA spectrum of lignin, vinyl- modified lignin in O_2.

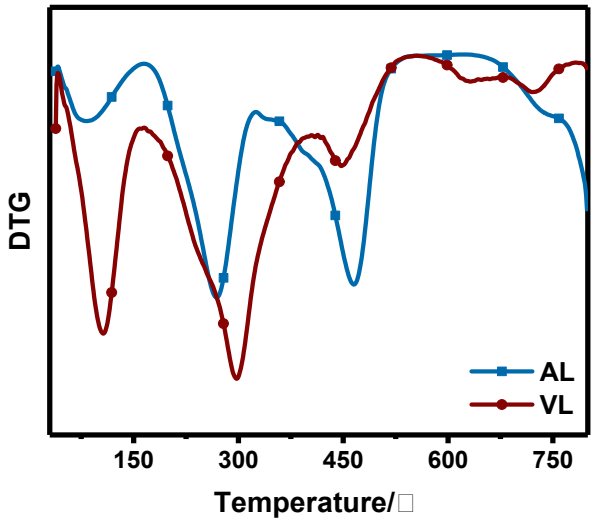

Fig.S7 DTG spectrum of lignin, vinyl- modified lignin in O_2

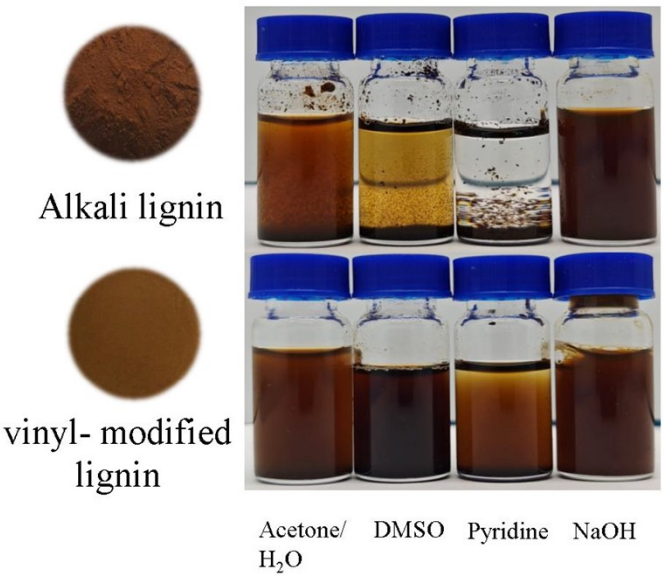

Fig. S8 Dissolution tests of Kraft lignin and Oz-L in acetone/ethanol (1:1, v/v), DMSO, pyridine and 2% NaOH.

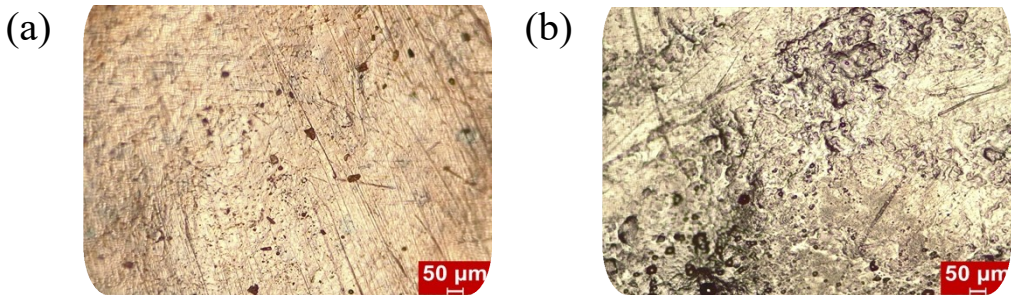

Fig. S9 Microscope images before and after EMTO-VL self-healing.

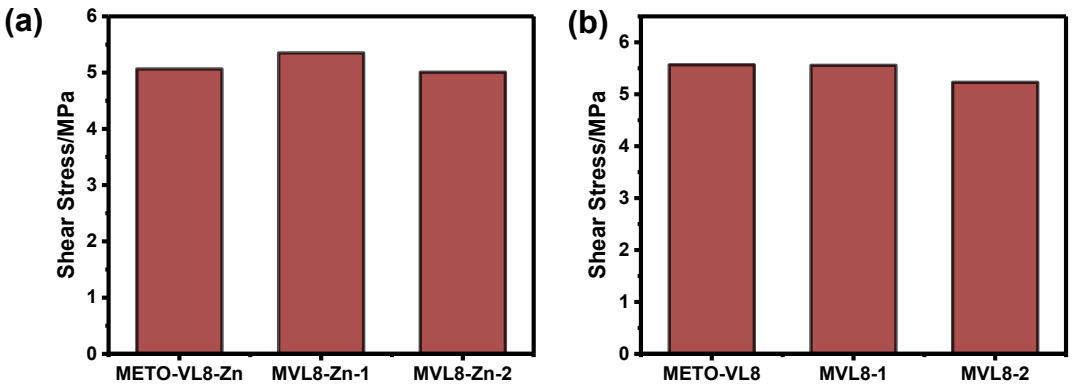

Fig. S10 (a) Shear strength of EMTO-VL_8 after different self-healing cycles. (b) Shear strength

of EMTO-VL_8-Zn^{2+} after different self-healing cycles.

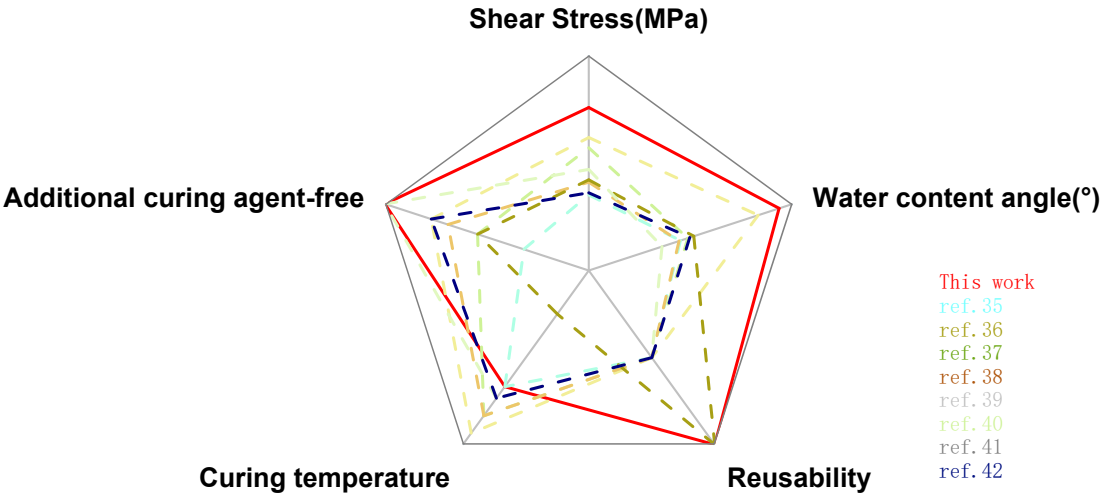

Fig.S11 Comparison of EMTO-VL adhesives with previously reported biomass adhesives in terms of shear strength, additional curing agent-free, reusability, water resistance, and curing temperature.

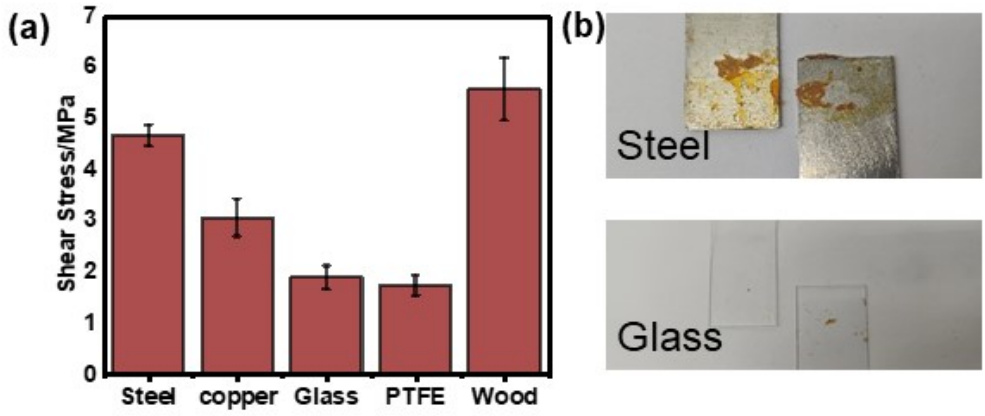

Fig.S12 (a) The shear strength of EMTO-VL8 on different substrate surfaces. (b) Microscope image of EMTO-VL8 after bonding Steel and Glass.