

EFFICIENT-RATIONALLY PREDICTING AND SYNTHESIZING INTRINSIC HIGH FIRE-SAFETY POLYCARBONATE WITH PROCESSABILITY

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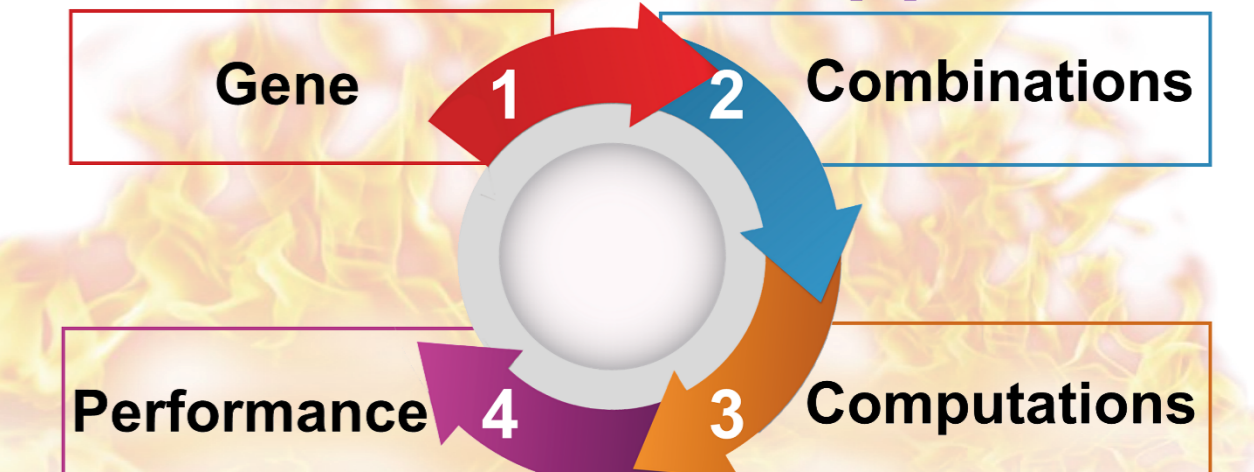
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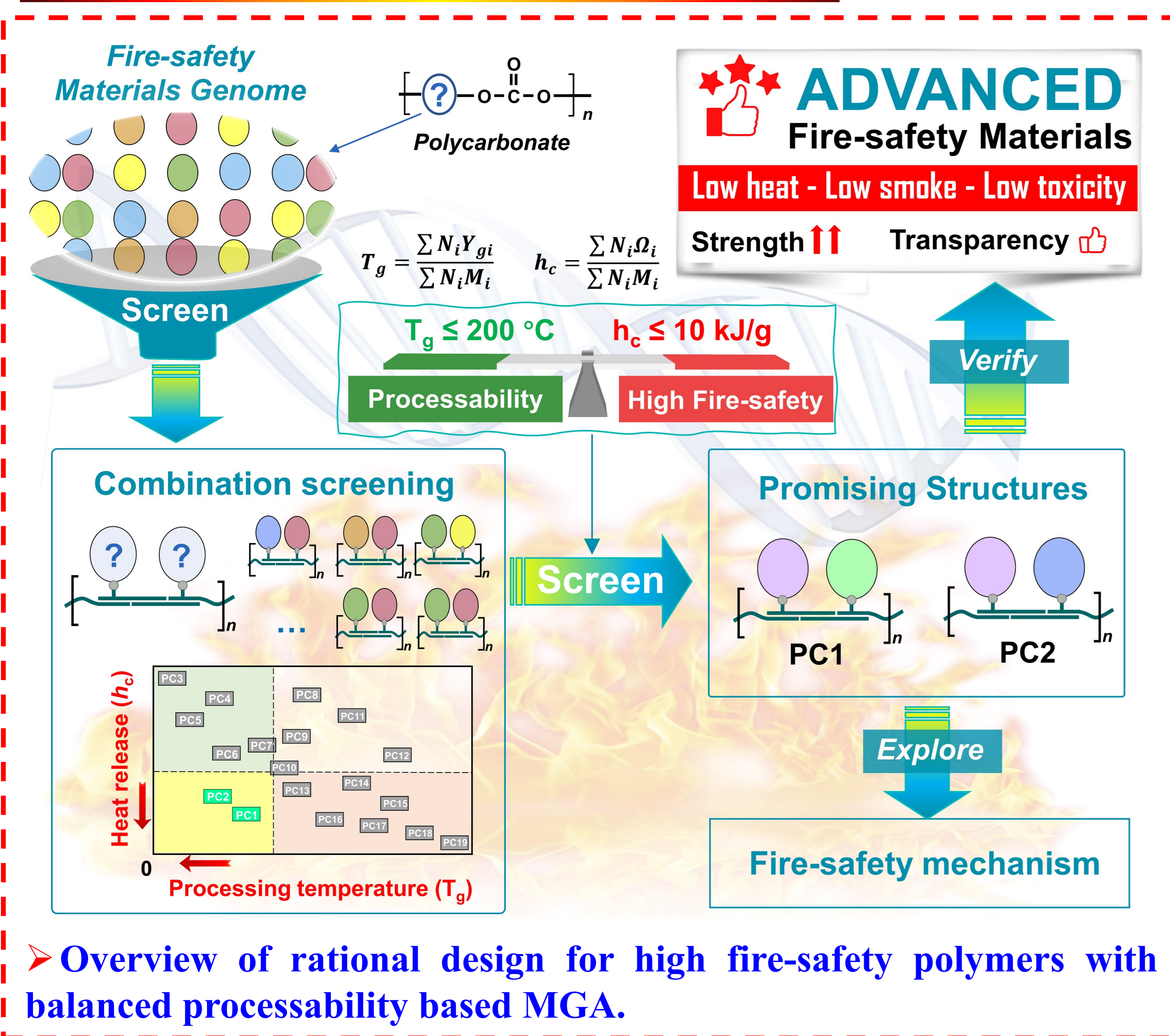
Background

High fire-safety is extremely required for polymer materials applied in many social environments, but the contradiction between fire-safety and processability for molecular design of intrinsic high fire-safety polymers has remained a challenge. The traditional design based on scientific intuition and trial-and-error experimentation is time-consuming and rather inefficient, herein, we established a simple material genome approach (MGA) allowing high-throughput screening of intrinsic fire-safety and processable polycarbonate (PC).

Material Genome Approach



1. Research Strategy



➤ Overview of rational design for high fire-safety polymers with balanced processability based MGA.

2. Results and Discussion

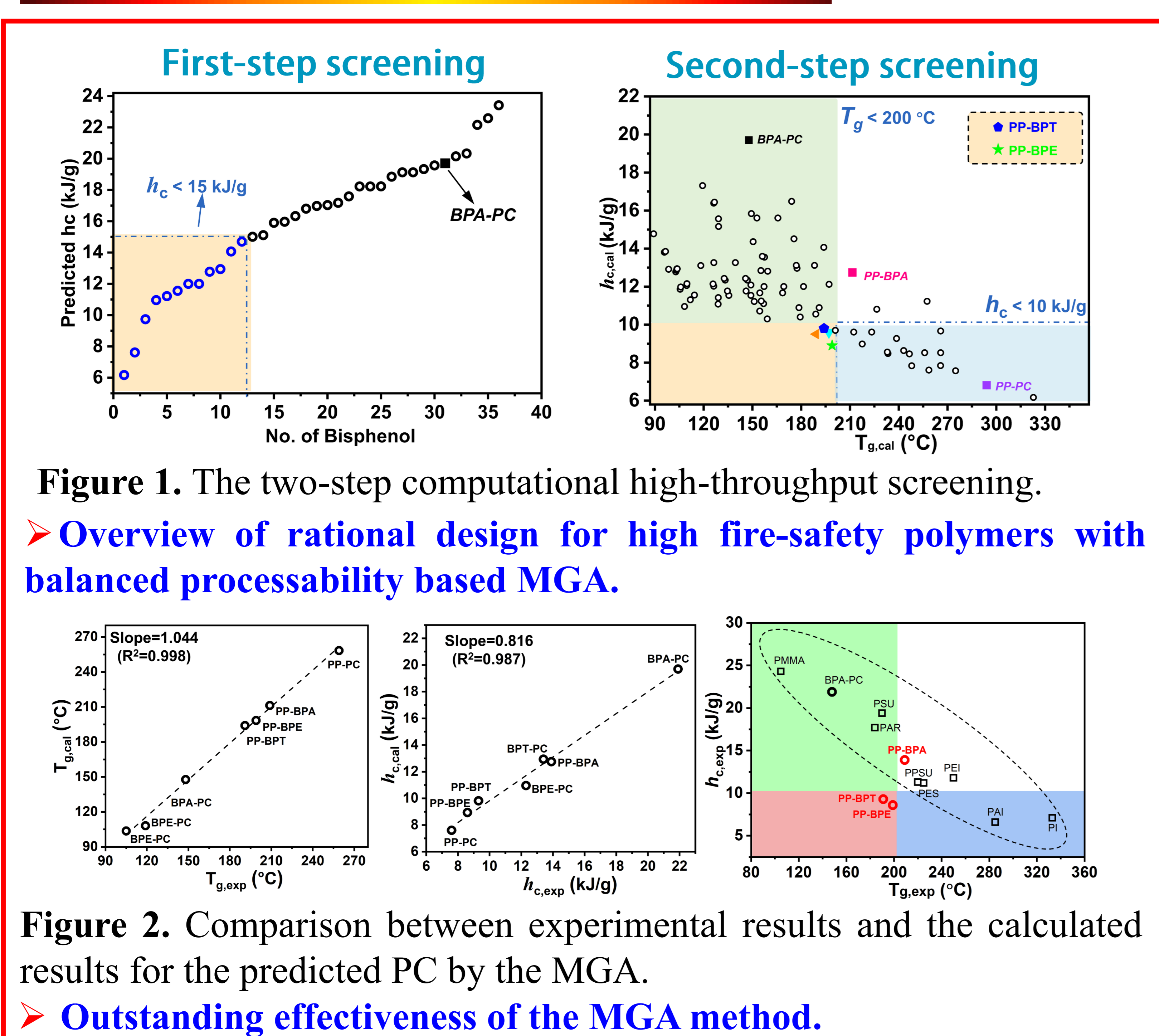


Figure 1. The two-step computational high-throughput screening.

➤ Overview of rational design for high fire-safety polymers with balanced processability based MGA.

Figure 2. Comparison between experimental results and the calculated results for the predicted PC by the MGA.

➤ Outstanding effectiveness of the MGA method.

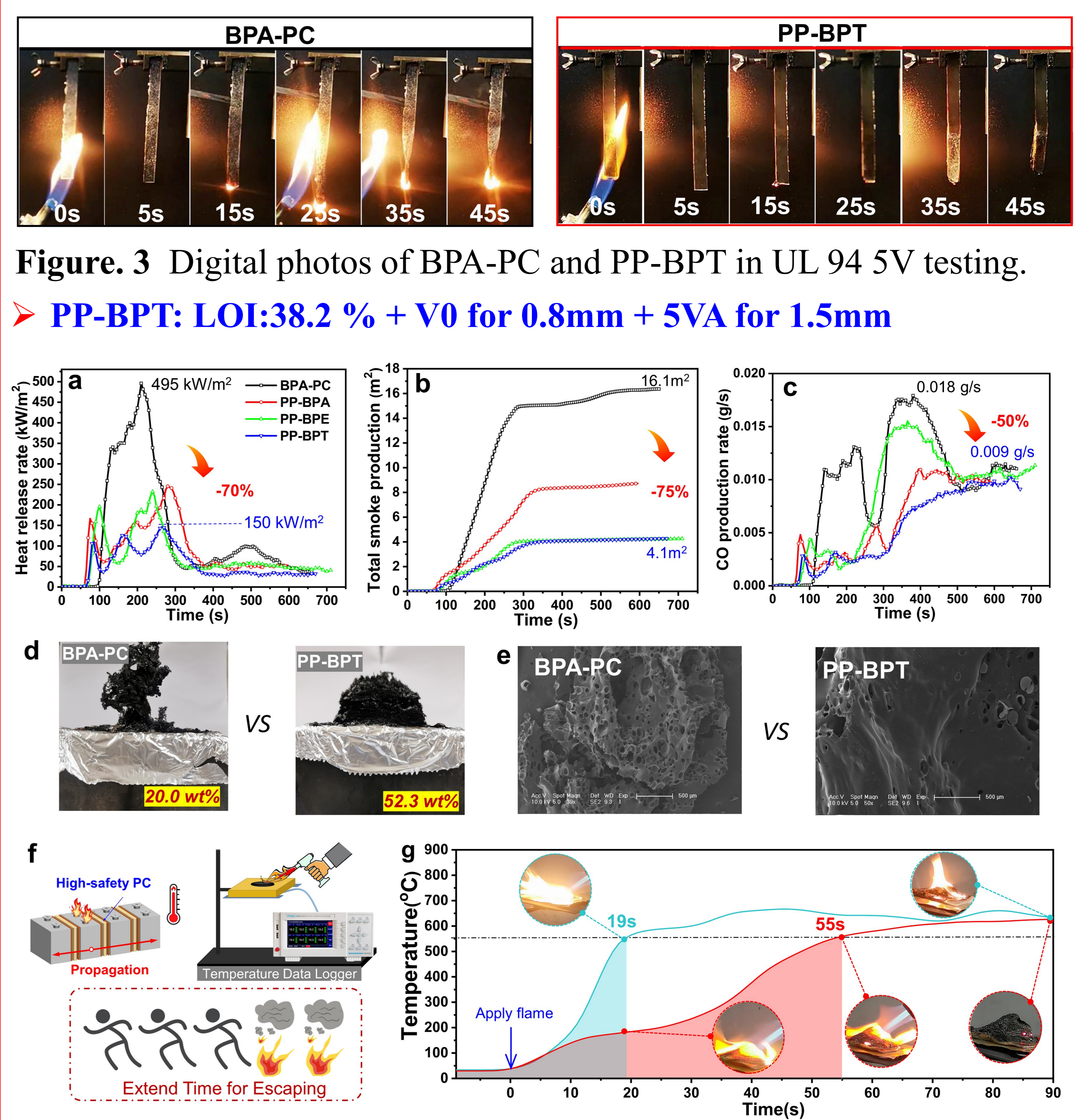


Figure 4. The results of cone calorimeter and thermal insulated tests.

➤ Low heat / Low smoke / Low toxicity / High efficient carbonization.
➤ The char of PP-BPT was denser and had better barrier effect.

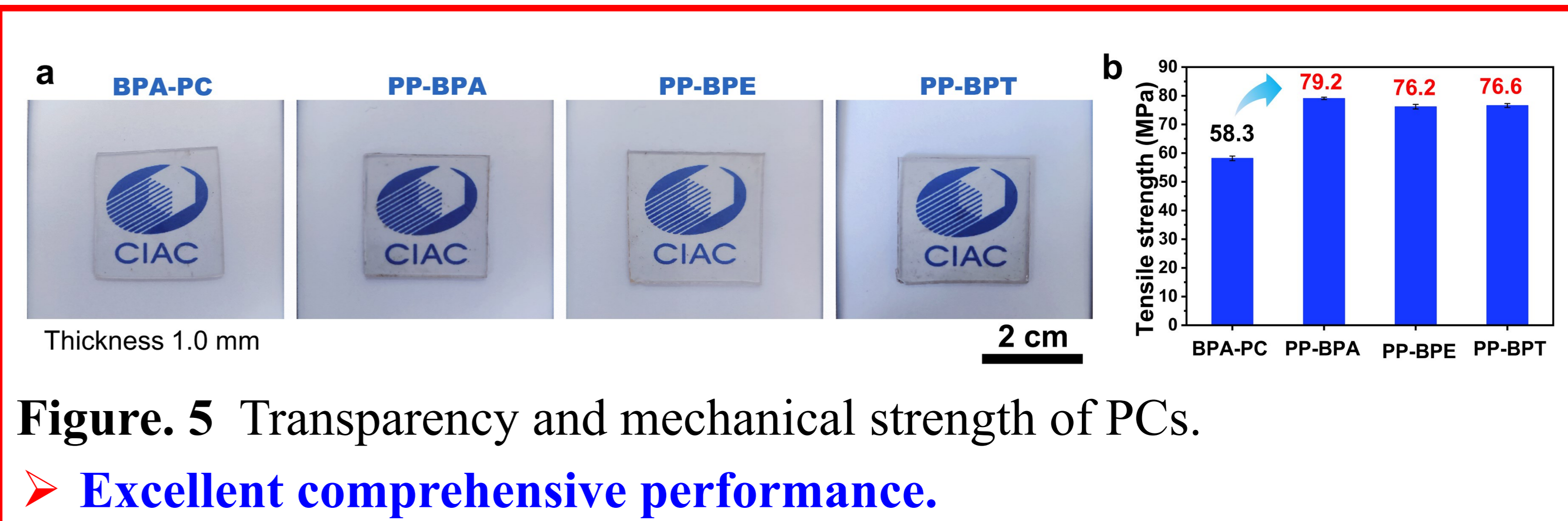


Figure 5. Transparency and mechanical strength of PCs.

➤ Excellent comprehensive performance.

3. Conclusion

- ◆ A material genome approach (MGA) has been successfully established in this work to rapidly screen processable high fire-safety polycarbonates.
- ◆ The agreement between theoretical calculations and experimental values confirms the excellent effectiveness of the MGA method.
- ◆ This work will provide a novel opportunity in the synthesis and applications of high fire-safety polymers.