

Self-assembly and Hydrogelation from Multicomponent Coassembly of Pentafluorobenzyl-phenylalanine and Pentafluorobenzyl-diphenylalanine

Shu-Min Hsu, Fang-Yi Wu, Zong-Sheng Lai, Yu-Chun Lin and Hsin-Chieh Lin*
Department of Materials Science and Engineering, National Chiao Tung
University, Hsinchu, 300, Taiwan, Republic of China

Supporting Information

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Materials: The amino-acid derivative of PFB-F and peptide derivative of PFB-FF were synthesized as described in our previous report.^{S1} The PFB-F and PFB-FF were prepared by solid phase peptide synthesis (SPPS) using 2-chlorotrityl chloride resin (100-200 mesh and 0.3-0.8 mmol/g).

Hydrogel preparation: Gelation was performed by weighing a compound (2.0 mg) in a screw-capped 2-mL vial (diameter: 10 mm). Sodium hydroxide solution was added to the suspension to adjust pH; alternating vortex and ultrasonication were applied until a clear solution was obtained. This solution was then neutralized by a dropwise addition of hydrochloric acid for gelation.

Transmission Electron Microscopy: Images were obtained with a Hitachi HT7700 transmission electron microscope at an accelerating voltage of 100 kV. Hydrogels were applied directly onto 200 mesh carbon-coated copper grids. Excess amount of the hydrogel was carefully removed by capillary action (filter paper), and the grids were then immediately stained with uranyl acetate for 30 s. Excess stain was removed by capillary action, and the grids were allowed to air dry.

Rheological tests: Rheological tests were conducted using an Anton Paar rheometer and a 25-mm parallel plate. The hydrogel sample (400 μ L, 1 wt %) was placed on the parallel plate for the angular frequency sweep test (test range: 0.25 to 100 rads^{-1} ; 13 points per decade; sweep mode, “log”; temperature, 25 $^{\circ}\text{C}$) and oscillatory strain (test range: 0.1% to 15%; frequency, 1 rads^{-1} ; 21 points per decade; sweep mode, “log”; temperature, 25 $^{\circ}\text{C}$).

Cell viability tests: The biocompatibilities of different peptides were measured by the MTT cell viability test. The CTX TNA2 and MCF-7 cells were seeded in 24-well plates at a density of 50000 cells per well with 0.5 mL medium (DMEM) contained 10% FBS and 1 % Penicillin-streptomycin solution and incubated for 24 h. Compounds at different concentrations (10, 50, 100, 200, 500 μM) were added when cells were plated. 24, 48 and 72 h later, replaced the medium with fresh medium supplemented with 0.5 mL of MTT reagent (4 mg mL^{-1}) per well. After another 4 h, the medium containing MTT was removed and DMSO (0.5 mL per well) was added to dissolve the formazan crystals. Each 24-well was transferred to 96 well plate. The optical density of the result solution was measured at 595 nm, using an absorbance microplate reader (Infinite F50, TECAN). Cells without the treatment of the compounds were used as the control. The cell viability percentage was calculated by the following formula: The cell viability percentage (%) = $\text{OD}_{\text{sample}}/\text{OD}_{\text{control}}$.

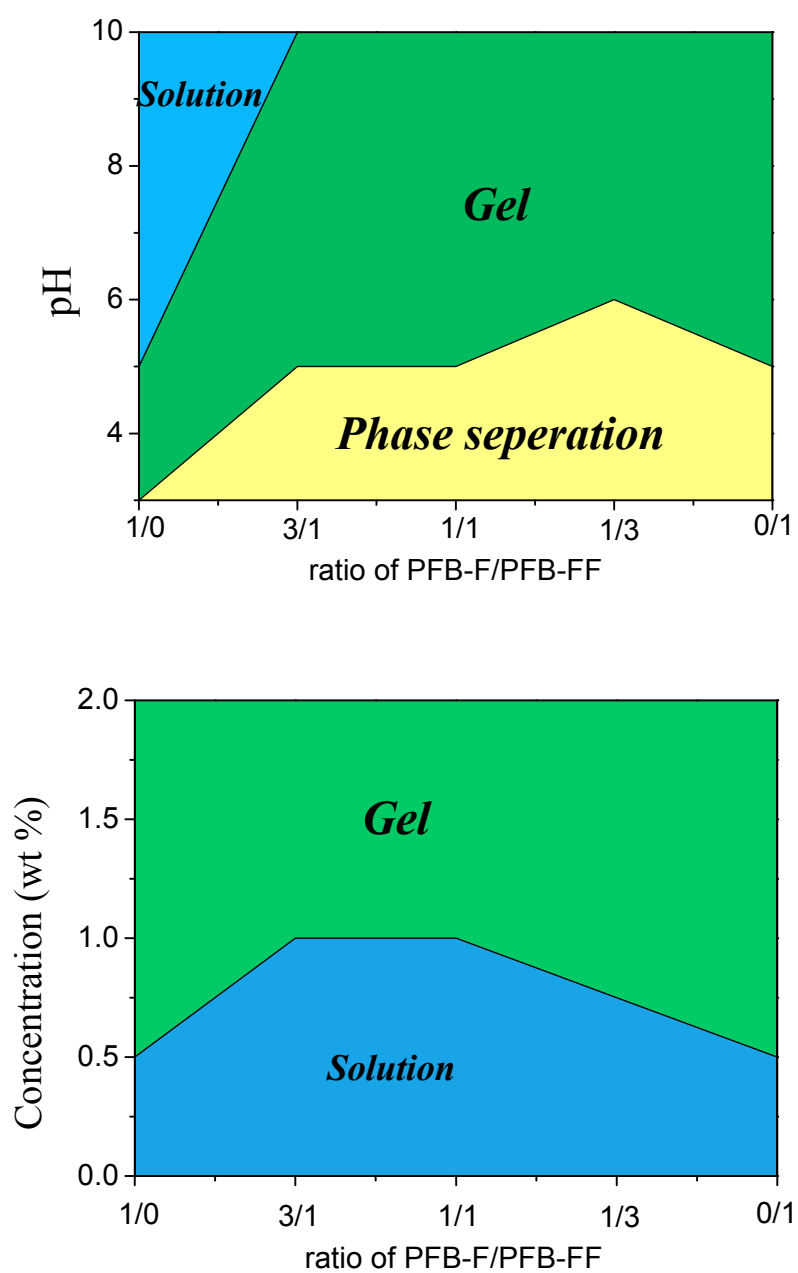


Fig. S1. Gelation behaviors of the systems: (upper) pH values versus various ratios of PFB-F and PFB-FF and (lower) concentrations versus ratios of PFB-F and PFB-FF.

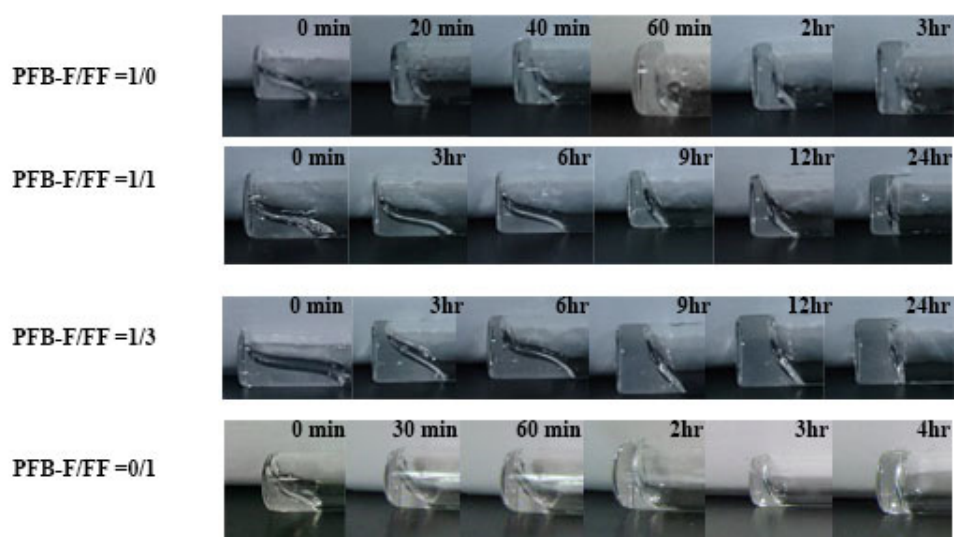


Fig. S2. Gelation behaviors of the systems as a function of time. Note that the gelation time of PFB-F/FF=3/1 is longer than 4 days (5-7 days).

Reference:

S1 S.-M. Hsu, Y.-C. Lin, J.-W. Chang, Y.-H. Liu, and H.-C. Lin, *Angew. Chem. Int. Ed.*, 2014, **53**, 1921-1927.