Self-assembly of Chiral (1R,2S)-Ephedrine and (1S,2S)-Pseudoephedrine into Low-dimensional Aluminophosphate Materials Driven by their Amphiphilic Nature

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Supporting Information

Details of the Solid State MAS NMR Spectroscopy

Solid State MAS NMR measurements were recorded on a Bruker AV-400-WB spectrometer. ^{19}F one-pulse MAS spectra were collected using $\pi/2$ (2 μs) rad pulses, 300 kHz spectral width and 120 s recycle delays; the spinning speed was set at 20 kHz. ^{27}Al experiments were carried out in a 4mm triple resonance probe, using a $\pi/30$ (0.4 μs, 30 kHz) pulse, 50 kHz spectral width, 0.5 s relaxation delay and 4k transients; samples were spun at 10 kHz. ^{1}H to ^{13}C Cross-Polarization spectra were recorded using $\pi/2$ rad pulses of 4.5 μs for ^{1}H, a contact time of 5 ms and a recycle delay of 3 s. For the acquisition of the ^{13}C spectra, the samples were span at a rate of 5-5.5 kHz. For ^{31}P, $\pi/2$ rad pulses of 4.25 μs and recycle delays of 80 s were used; these spectra were recorded while spinning the samples at ca. 11 kHz.

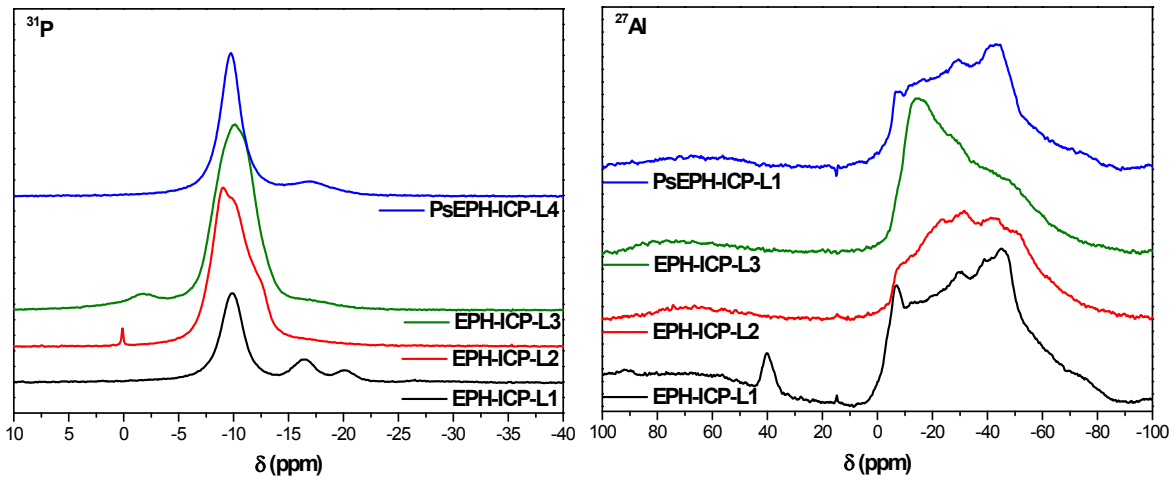

Figure S1. ^{31}P MAS NMR of low-dimensional materials obtained with EPH or PsEPH.

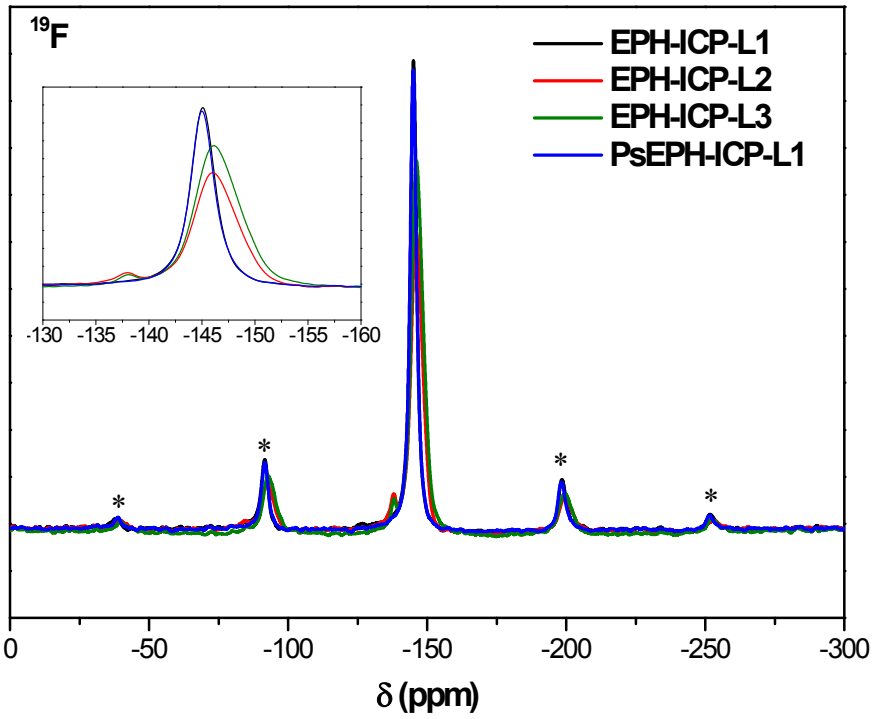

Figure S2. ^{19}F MAS NMR of low-dimensional materials obtained with EPH or PsEPH.

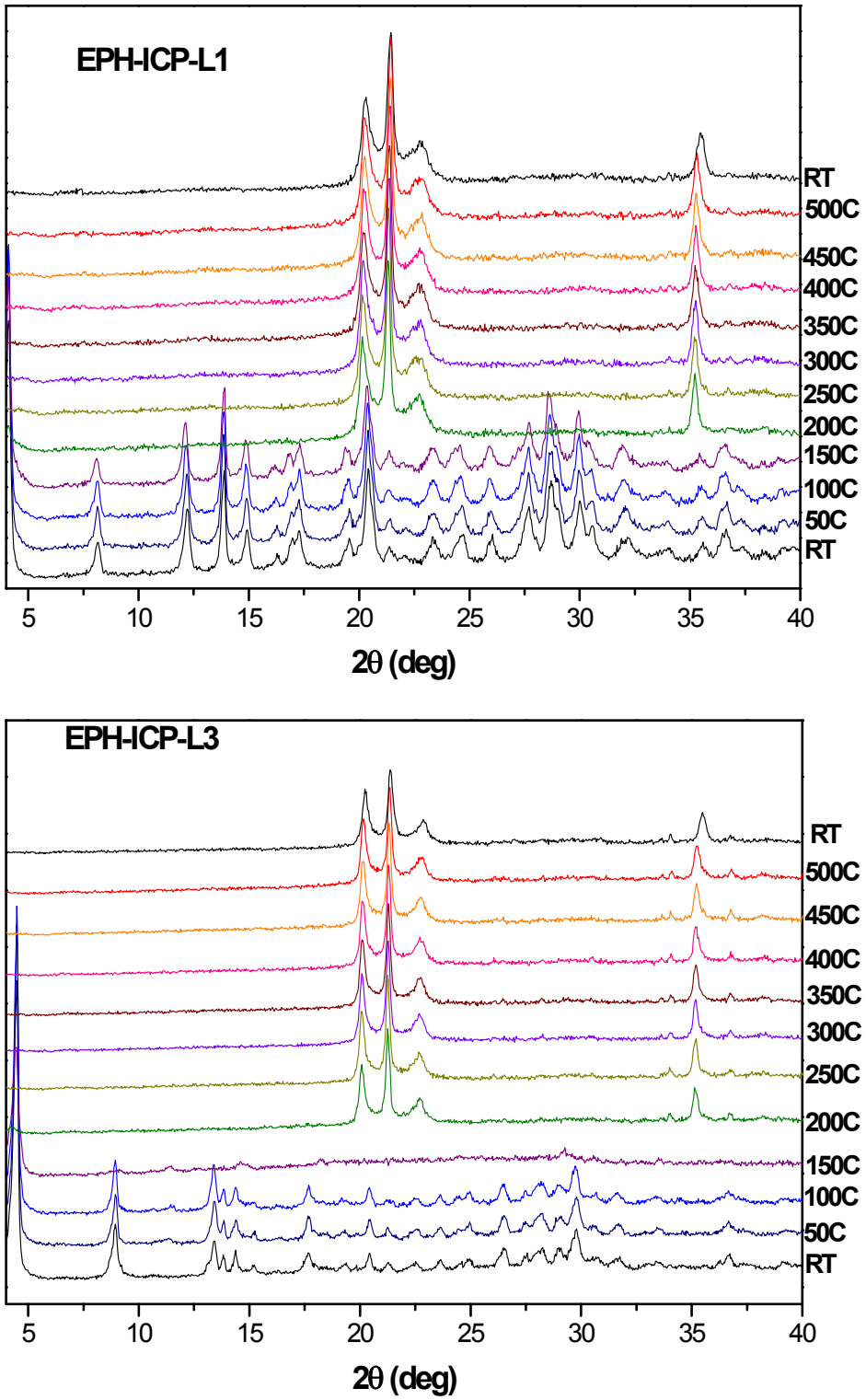

Figure S3. In-situ XRD patterns at increasing temperatures of EPH-ICP-L1 (top) and EPH-ICP-L3 (bottom).

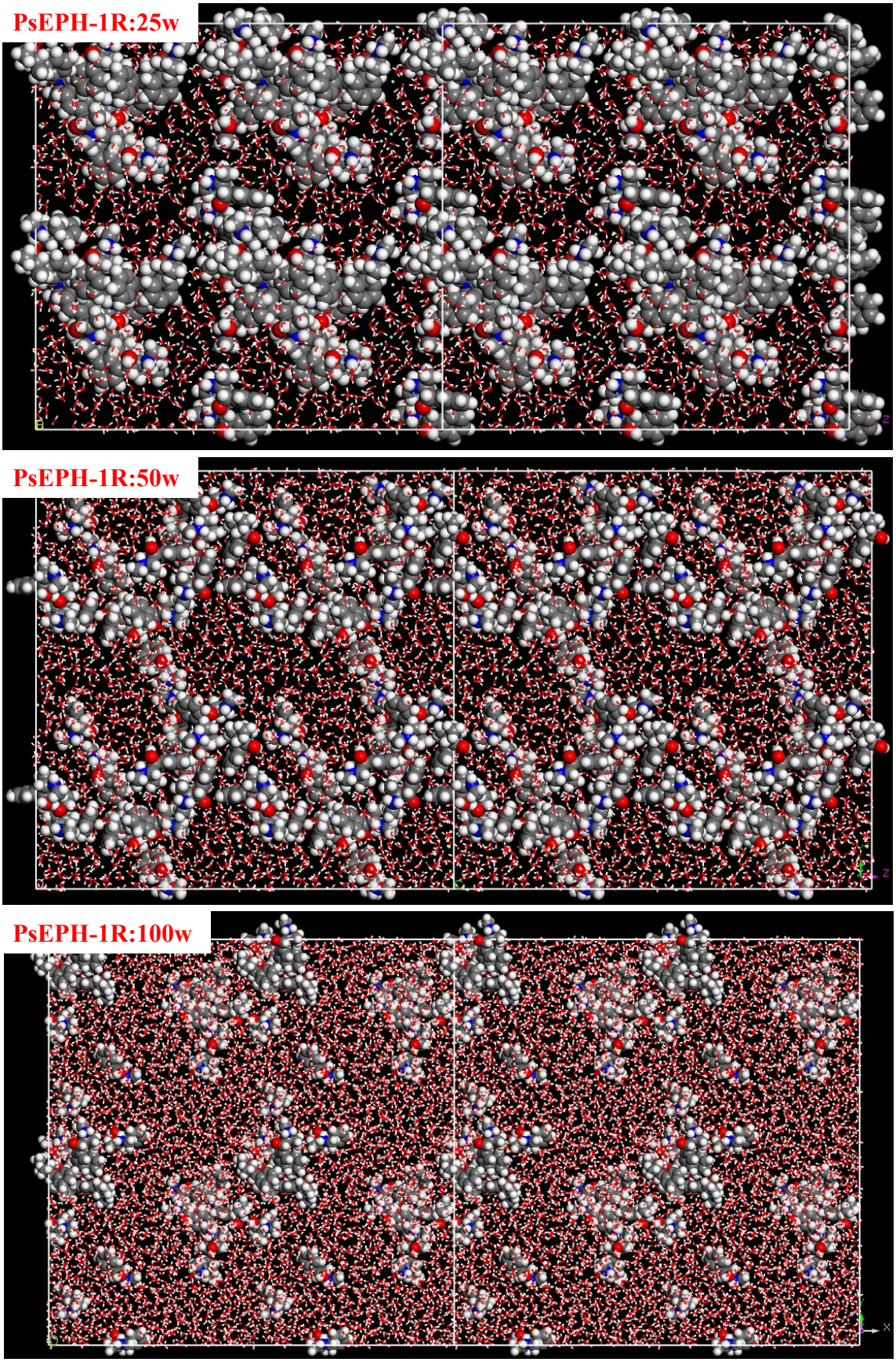

Figure S4. Snapshot (MD t = 1000 ps) of the aggregation of PsEPH at the different concentrations; EPH molecules are shown as CPK models, and water molecules as line models.

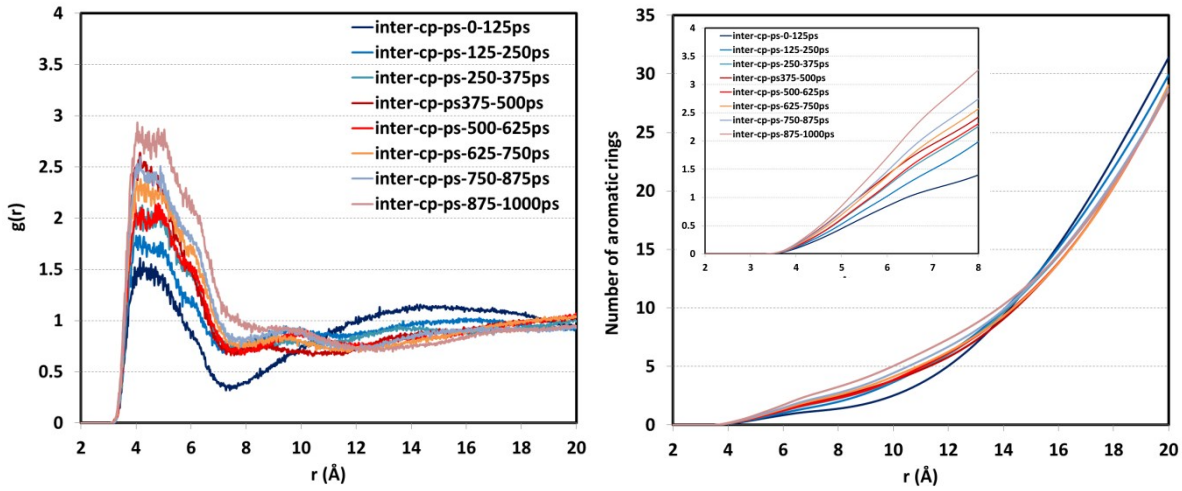

Figure S5. Evolution of the RDF between aromatic C atoms (calculated in different time intervals) (left) and of the corresponding concentration profiles (right) for EPH at 1R:25H_2O composition.

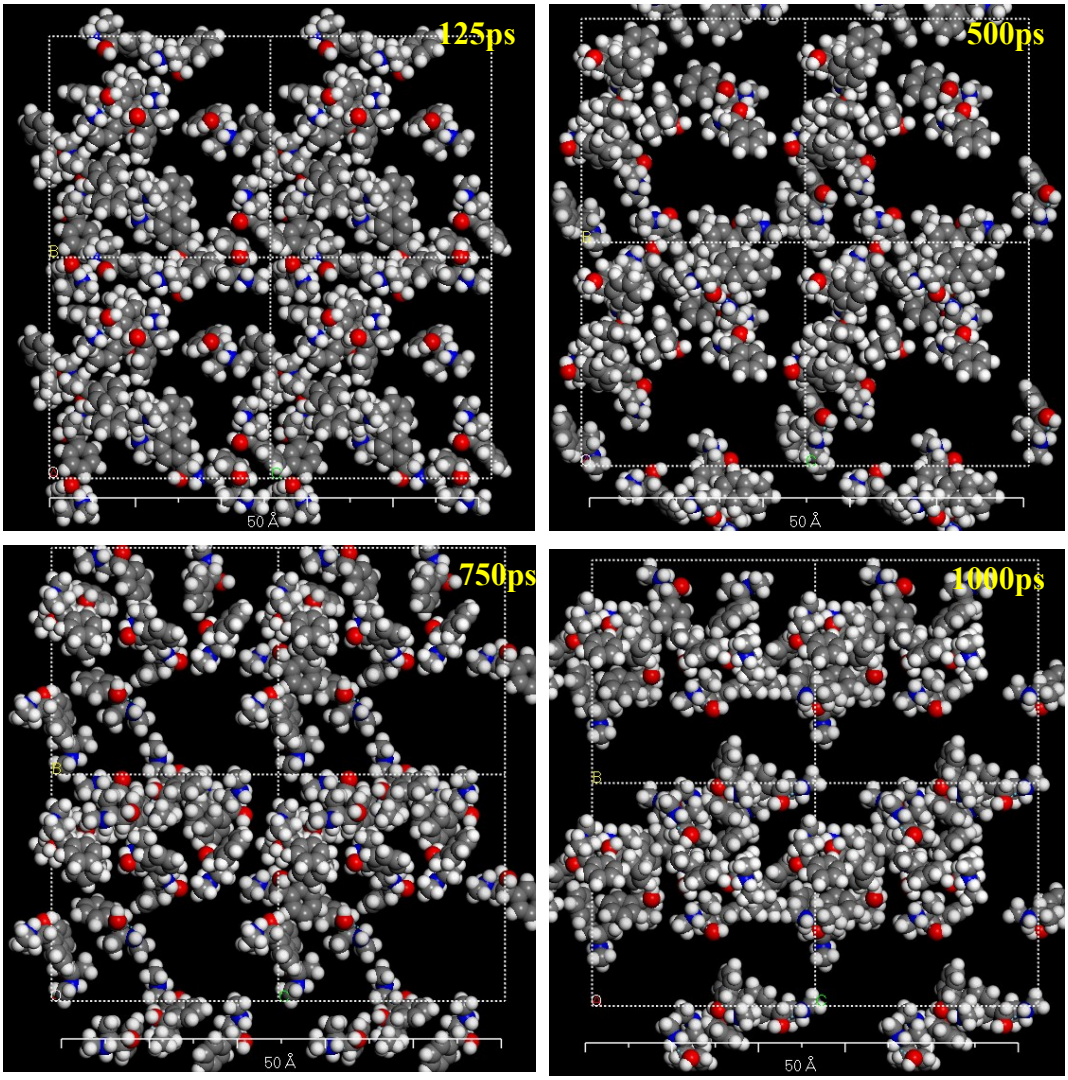

Figure S6. Snapshots (at different MD times) showing the evolution of the supramolecular aggregation of EPH molecules at 1R:25H_2O composition.

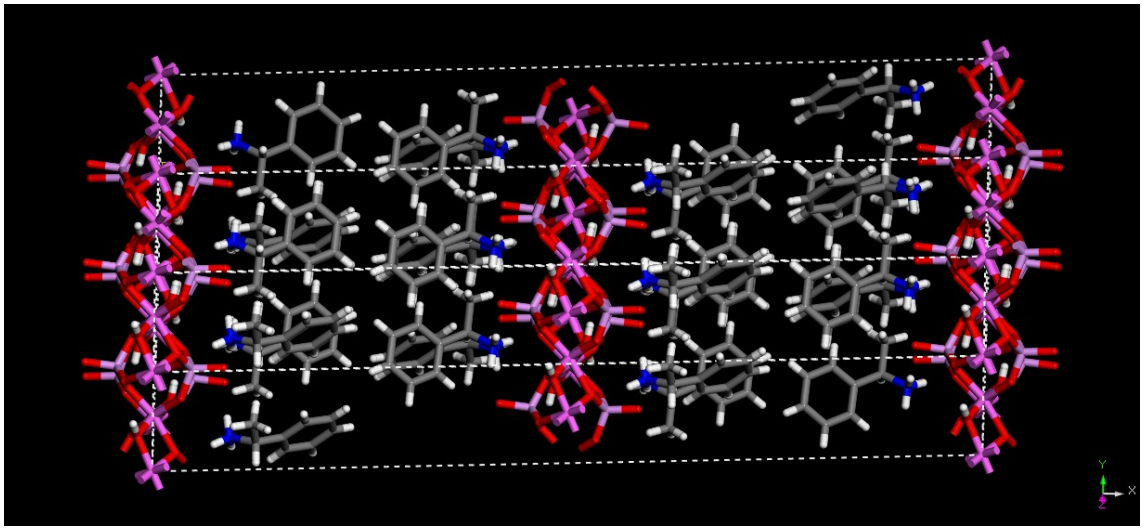

Figure S7. Structure of a layered material formed by an organic bilayer through supramolecular aggregation, without showing π-π stacking interactions.