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Effect of strand register in the stability and reactivity of crystals from peptides forming amyloid fibrils

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Figures

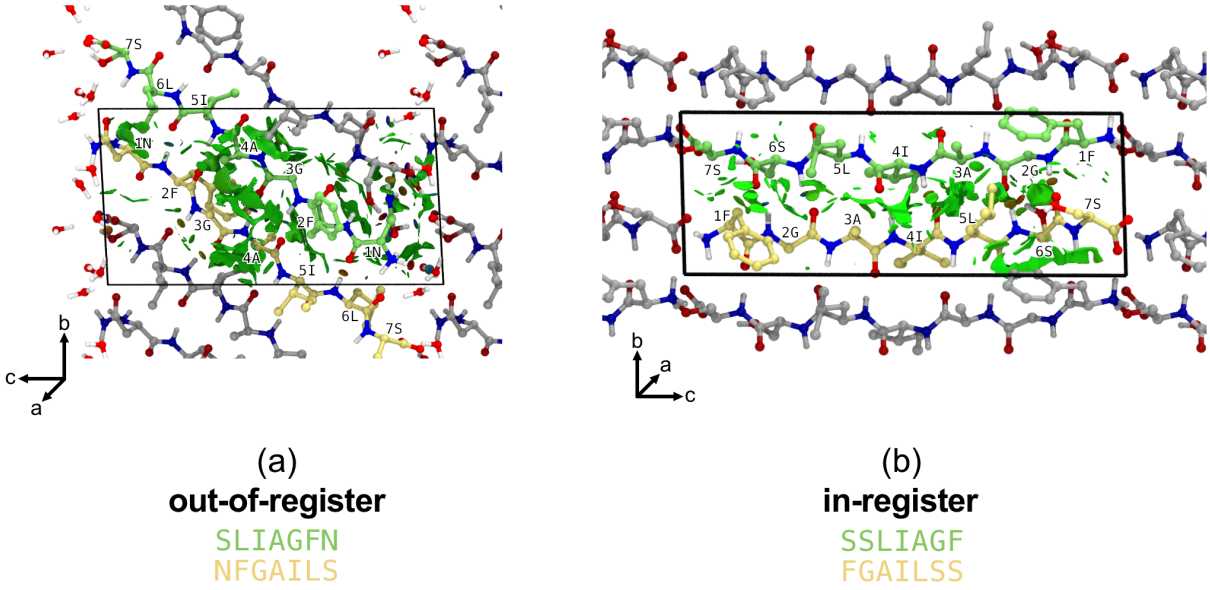

Figure S1: Noncovalent interaction (NCI) analysis of the crystals `NFGAILS` (out-of-register) and `FGAILSS` (in-register). Peptide units forming the β-strand dimer are colored in yellow and green. Hydrogen atoms of polar groups are shown only for clarity. Amino acids are labeled by their sequence number and one-letter code. NCI surfaces are colored using a red-green-blue scheme for repulsive, weak, and attractive forces, respectively.

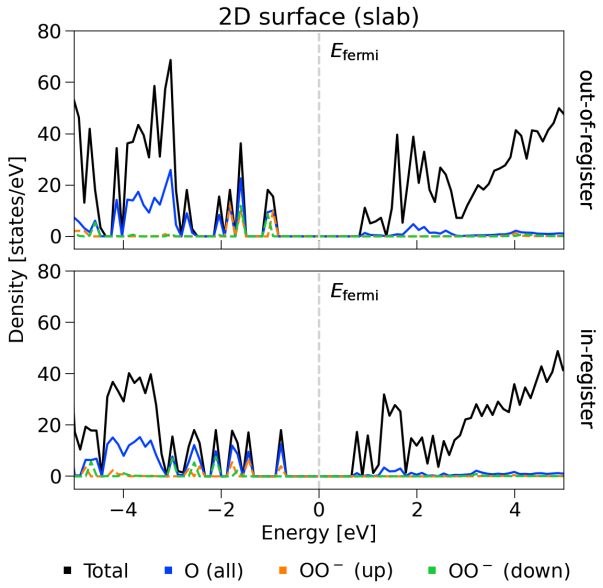

Figure S2: Density of states (DOS) and partial DOS (PDOS) of the out-of-register and in-register peptide slabs. DOS is shown in black, PDOS of all oxygen atoms in blue, and PDOS of the carboxylate oxygen atoms at the up and down faces (refer to Figure 5) in orange and green, respectively. Energies are normalized to the Fermi level.

Tables

Table S1: Optimized lattice parameters, in Å and degrees, for peptide crystals.

Crystal	parameter	calculated	expt.	% error
	a	8.497	8.661	1.891
	b	11.560	11.594	0.290
NFGAILS	c	21.640	21.552	0.410
(5E5V)	α	85.149	86.389	1.435
	β	81.972	82.209	0.289
	γ	76.480	76.349	0.172
	a	8.598	8.770	1.960
	b	9.475	9.500	0.260
FGAILSS	c	24.543	24.740	0.795
(5E61)	α	88.599	88.220	0.429
	β	81.345	80.000	1.681
	γ	70.019	70.339	0.455