Amino acid derivatives of perylenediimide and their N–H···O peptide bond dipoles-templated solid state assembly into stacks

Cyprien Lemouchi, Sergey Simonov, Leokadiya Zorina, Christelle Gautier, Piétrick Hudhomme and Patrick Batail

Figure S1. UV-visible absorption spectra for dichloromethane solutions of 2a-b and tetrahydrofurane solutions of 1.

Figure S2. Cyclic voltammograms of compounds 2a and 2b and CV of precursor 1.

Figure S3. Molecular conformations of PDI-(Cl4)-[Gly-Ala(OEt)]2, 2a (Fig. S3a) and PDI-(Cl4)-[Gly-Val(OEt)]2, 2b (Fig. S3b) in solid state.

Figure S4. Overlap modes for (a) PDI-(Cl4)-[C2H4OH][4-(n-C5H11)]; (b) PDI-(Cl4)-[4-(n-C12H25)C6H4]; (c) PDI-(Cl4)-[Gly-Ala(OEt)]2, 2a; and (d) PDI-(Cl4)-[Gly-Val(OEt)]2, 2b.
(2a) \( C = 1.19 \times 10^{-5} \text{ mol.L}^{-1} \)

(2b) \( C = 2.23 \times 10^{-5} \text{ mol.L}^{-1} \)
Figure S1. UV-visible absorption spectra for dichloromethane solutions of 2a-b and tetrahydrofuran solutions of 1.

(1) \( C = 3.71 \times 10^{-5} \text{ mol.L}^{-1} \)
Electrochemical experiments were carried out with a Biologic SP-150 potentiostat at 293 K. Cyclic voltammetry was performed in a three-electrode cell equipped with a platinum-plate counter electrode and a platinum working electrode (0.125 cm$^2$). Reference electrode was Ag/AgNO$_3$ (0.01 M CH$_3$CN) and all the potentials are reported vs. Fc$^+/Fc$.

Figure S2. (A) Cyclic voltammograms (CVs) of compounds 2a (solid line) and 2b (dash line) in 0.1 M nBu$_4$NPF$_6$/CH$_2$Cl$_2$, (B) CV of precursor 1 in 0.1 M nBu$_4$NPF$_6$/THF. All CVs were performed at 0.1 V s$^{-1}$. 
Figure S3. Molecular conformations of PDI-(Cl₄)-[Gly-Ala(OEt)]₂, 2a (Fig. S3a) and PDI-(Cl₄)-[Gly-Val(OEt)]₂, 2b (Fig. S3b) in the solid state.
Figure S3. Overlap modes for (a) PDI-(Cl4)-[C2H4OH][4-(n-C5H11)]; (b) PDI-(Cl4)-[4-(n-C12H25)C6H4]; (c) PDI-(Cl4)-[Gly-Ala(OEt)]2, 2a; and (d) PDI-(Cl4)-[Gly-Val(OEt)]2, 2b.