Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Why do Polyarginines Adsorb at Neutral Phospholipid Bilayers and Polylysines do not? An Insight from Density Functional Calculations and Molecular Dynamics Simulations

Carmelo Tempra,[1] Zlatko Brkljača,[2,a] Mario Vazdar[3,*]

[a)] Present address: Selvita d.o.o. Prilaz baruna Filipovića 29, 10000 Zagreb, Croatia.

[1]Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 542/2, 16000 Prague, Czech Republic

[2]Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, Croatia

[3]Department of Mathematics, Informatics and Cybernetics, University of Chemistry and Technology, Technická 5, 16628 Prague, Czech Republic

Corresponding author e-mail: mario.vazdar@vscht.cz

Supplementary Information

Page 2. Partial charges of charged groups described with ProsECCo force field used in peptide/bilayer MD simulations.

Table S1: The partial charges in the ProsECCo force field of charged groups in POPC, POPE lipids, R_9, K_9 peptides, and Cl^- counterion.

	POPC lipid		POPE lipid		R_9/K_9 peptide			ions
Scaled groups	$2O(PO_4^-)$	choline	$2O(PO_4^-)$	NH_3^+	$-NH_2$	$-COO^-$	Gdm^+/NH_3^+	Cl^-
Partial charges	-0.655	+0.75	-0.655	+0.75	+0.75	-0.75	+0.75	-0.75