

# An Atomistic Study of a Poly(styrene sulfonate)/Poly(diallyldimethylammonium) Bilayer: The Role of Surface Properties and Charge Reversal

Baofu Qiao\*, Marcello Sega and Christian Holm\*

*Institute for Computational Physics, Universität Stuttgart, Pfaffenwaldring 27, 70569  
Stuttgart, Germany*

In Table S1, given are the average number of monomers adsorbed in the 1<sup>st</sup> and 2<sup>nd</sup> deposition cycles. The rinsed PSS monolayer was composing of the 1<sup>st</sup> deposition cycle. For the 2<sup>nd</sup> deposition cycle, only those monomers on strongly adsorbed PDADMA chains were taken into consideration. In the present work, a PDADMA chain is defined to be strongly adsorbed if at least one of its nitrogen atoms is located in the region of  $z \leq 2.5$  nm from the adsorbing surface (see Fig. 6 in the main text).

TABLE S1. Average number of adsorbed monomers in the 1<sup>st</sup>/2<sup>nd</sup> deposition cycle <sup>a</sup>

surface		$\langle N_{PSS} \rangle$	$\langle N_{PDADMA} \rangle$
P/H <sup>b</sup>	$Q_s$ <sup>c</sup>		
P	0	64	86
P	16	84	69
P	36	76	75
H	0	60	74
H	16	76	75
H	36	88	82

<sup>a</sup> The standard deviations are less than 20% of the corresponding average values.

<sup>b</sup> P/H represents system with hydroxylated/non-hydroxylated adsorbing surface, respectively.

<sup>c</sup> Number of surface charges (in unit of e).