

**TABLE 1. Tight-Binding Parameters  $\epsilon$  and  $t$  for Each Subunit (in eV)<sup>a</sup>**

subunit	site number	represent	$\epsilon$	$t, t_n$	$\epsilon$ (lit.)	$t$ (lit.)
$S_1$	1	thiol	-4.2	6, 6		
$S_2$	2-5	methylenes	-14	6	-13.9 <sup>a</sup>	6 <sup>b</sup> , 7.7 <sup>c</sup>
$S_3$	6-7	amide	-1.3, -1.8	0.5, 1.8		1.8 <sup>d</sup>
$S_4$	8-9	methylene	-14	6	-13.9 <sup>a</sup>	6 <sup>b</sup> , 7.7 <sup>c</sup>
$S_5$	10-13	saturated tail group R	-14	6	-13.9 <sup>a</sup>	6 <sup>b</sup> , 7.7 <sup>c</sup>
$S_5$	10-13	conjugated tail group R	3.5	4, 1	5.9 <sup>e</sup>	4 <sup>e</sup> , 3.6 <sup>a</sup>
$S_6$	14-N	$\text{Ga}_2\text{O}_3$	-4.5 to -11.5			

<sup>a</sup> Subunits of the same kind are coupled by  $t$ . The coupling of a subunit to a saturated C neighbour is  $t_n$ , provided the subunit itself is not a saturated C (including methylene). Literature parameters are presented from (a) Benkő *et al.*<sup>31</sup> (b) Xu *et al.*<sup>32</sup> (c) Wang *et al.*<sup>33</sup> (d) Murrell<sup>34</sup> and (e) Salem<sup>35</sup>  $t$  param-

# Charge Transport Across Insulating Article Self Assembled

**Raffaella Di Napoli**



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