Electronic Supplementary Material (ESI) for RSC Advances

Adsorption of TCNQH-functionalized quinonoid zwitterions on gold and graphene: evidence for dominant intermolecular interactions

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The orbital energies with respect to the vacuum level using the semi-empirical PM3 model for

a) methoxybenzyl-functionalized zwitterion $C_6H_2(\cdots NHR)_2(\cdots O)_2$, where R = $-CH_2-C_6H_4-OCH_3$:
-0.38799 LUMO (+2)
-0.46374 LUMO (+1)
-2.11035 LUMO (0)
-7.57282 HOMO (0)
-9.01096 HOMO (-1)
-9.10518 HOMO (-2)

b) TCNQH-functionalization (TCNQH = $(NC)_2CC_6H_4CH(CN)_2$) of (6Z)-4-(butylamino)-6-(butyliminio)-3-oxocyclohexa-1,4-dien-1-olate $C_6H_2(\cdots NHR)_2(\cdots O)_2$ (where R = *n*-C_4H_9):

-0.54888 LUMO (+2)
-0.73256 LUMO (+1)
-3.736 LUMO (0)
-8.60307 HOMO (0)
-9.53232 HOMO (-1)
-9.65609 HOMO (-2)