Supplementary Information

Charge Transport of Silicon (IV) and Zinc (II) Phthalocyanines by Molecular Junction Models

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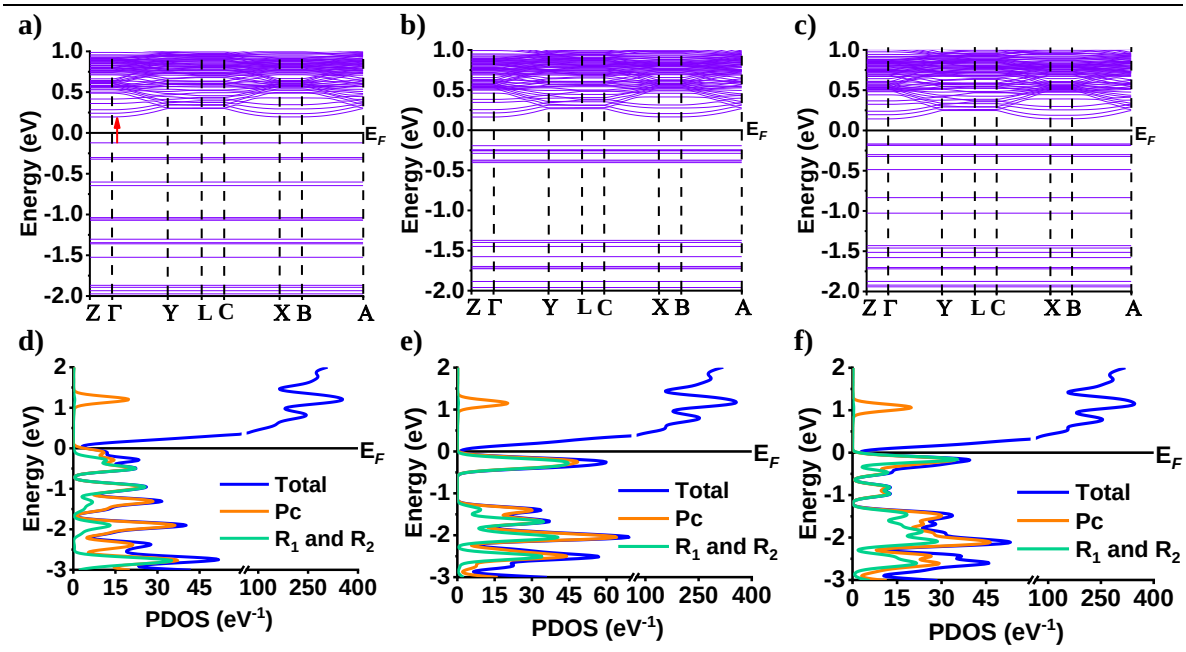


Figure S1. Electronic properties of systems adsorbed in TiO_2. **Top**: Band structures: **a) ZnPc-1B**, **b) ZnPc2B**, **c) ZnPc-3B**. **Bottom:** Total DOS (blue), projected density of states over *2p* orbitals of phthalocyanine (orange) and substituents (green): **d) ZnPc-1B**, **e) ZnPc2B**, **f) ZnPc-3B**.

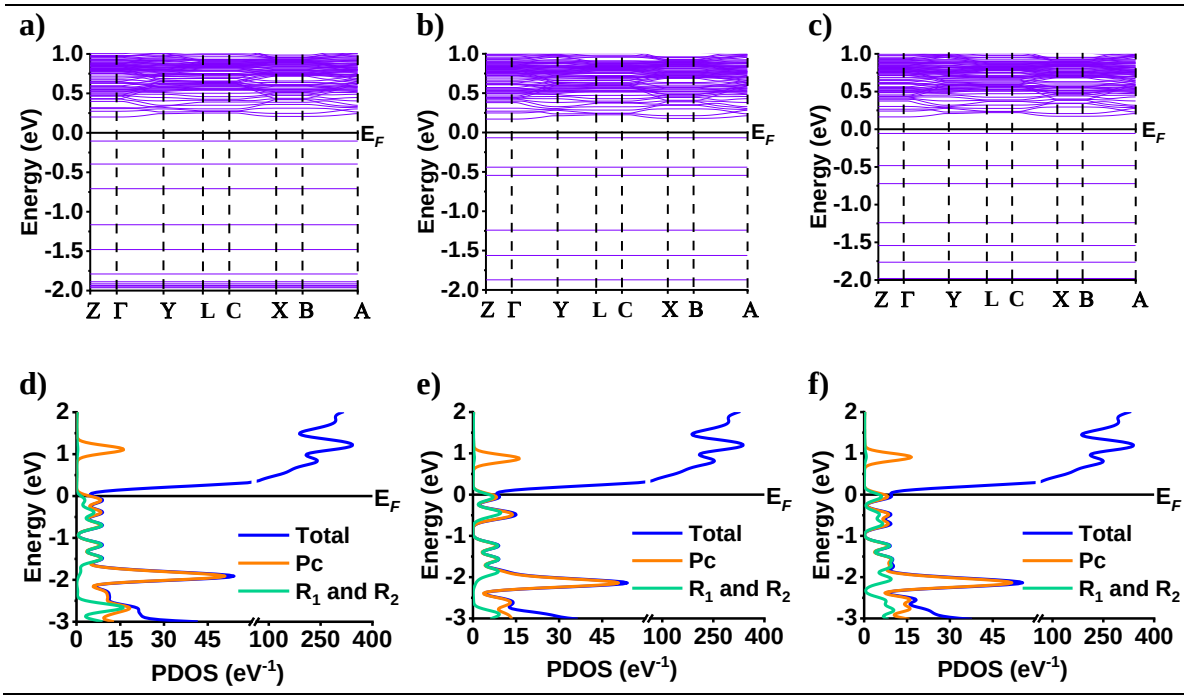


Figure S2. Electronic properties of systems adsorbed in TiO_2. **Top**: Band structures: **a) SiPc-1B**, **b) SiPc2B**, **c) SiPc-3B**. **Bottom:** Total DOS (blue), projected density of states over *2p* orbitals of phthalocyanine (orange) and substituents (green): **d) SiPc-1B**, **e) SiPc2B**, **f) SiPc-3B.**

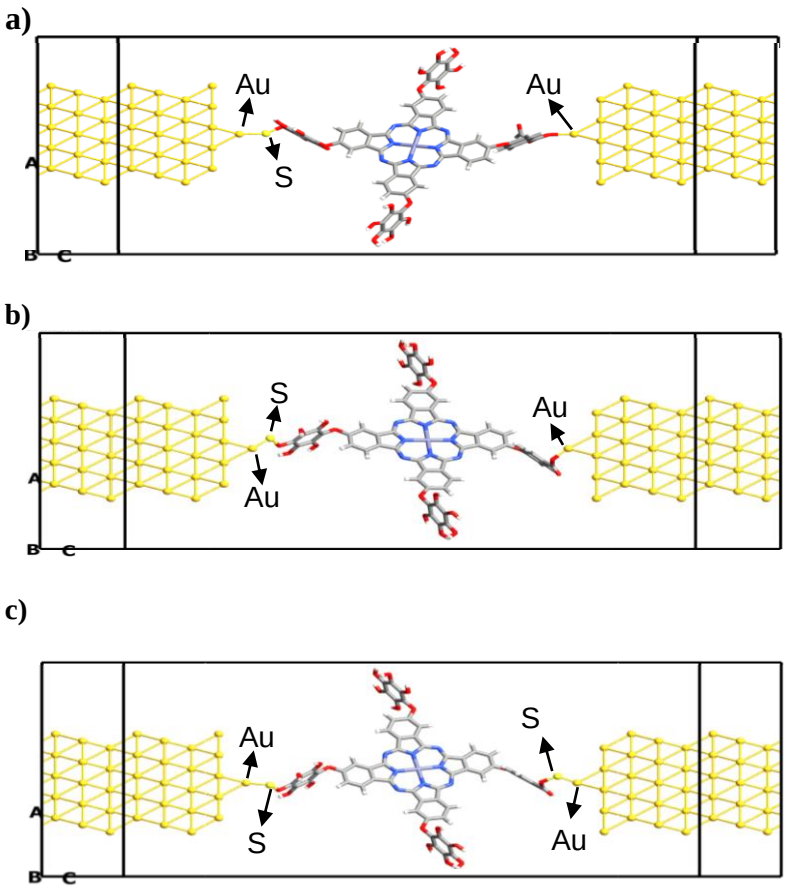
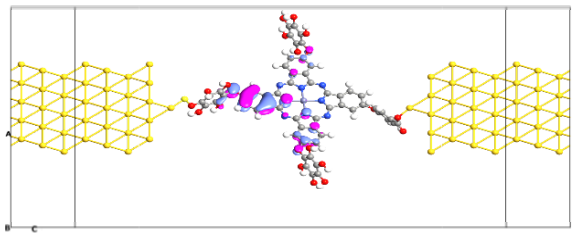
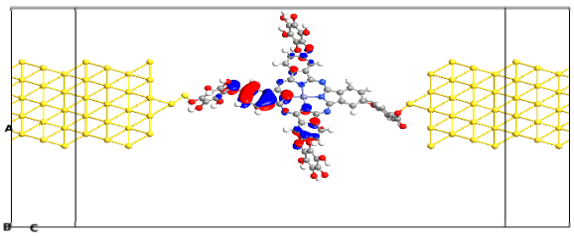


Figure S3. Molecular binding of **ZnPc-1A** toward the electrodes: **a)** Anhydrous group directly attached to the right electrode (**A**), **b)** Carboxyl group directly attached to the right electrode (**B1**), **c)** Carboxyl group bonded by sulfide bridges (**B2**) to the right Au (111) electrode.

ZnPc-1B1

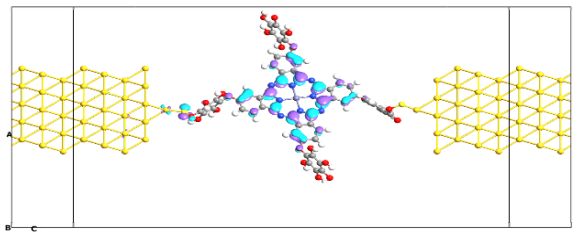


Transmission state = -1.24 eV



HOMO-6

ZnPc-1B2



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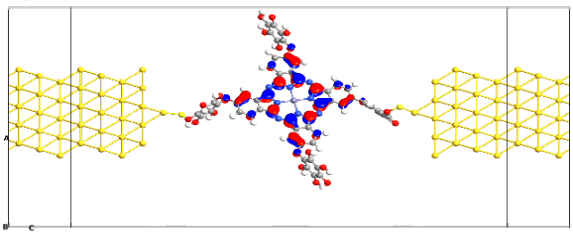
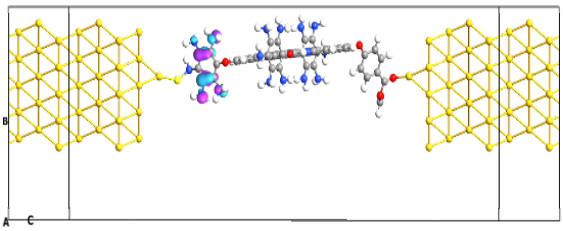
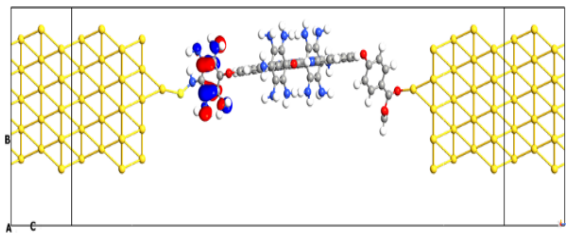


HOMO

ZnPc-2A

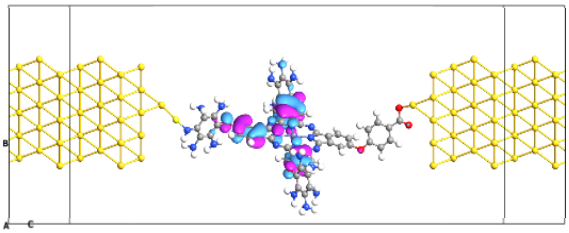


Transmission state = -0.344 eV



HOMO

ZnPc-2B1



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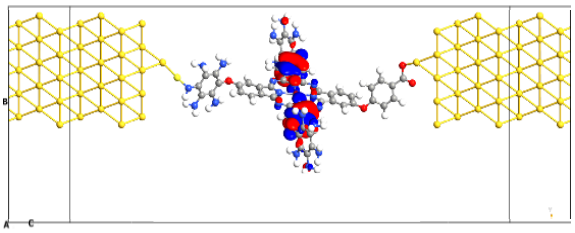
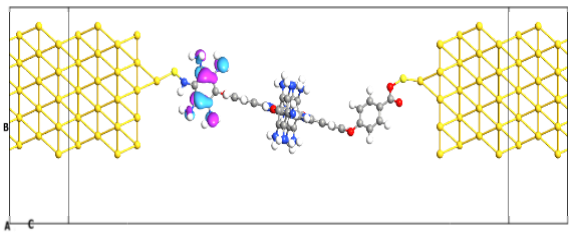
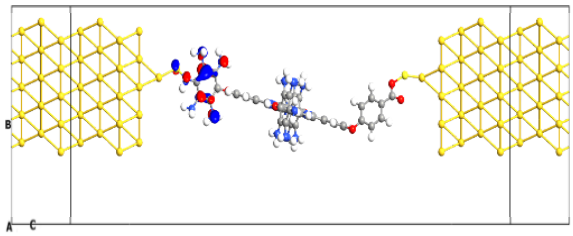


HOMO-8

ZnPc-2B2

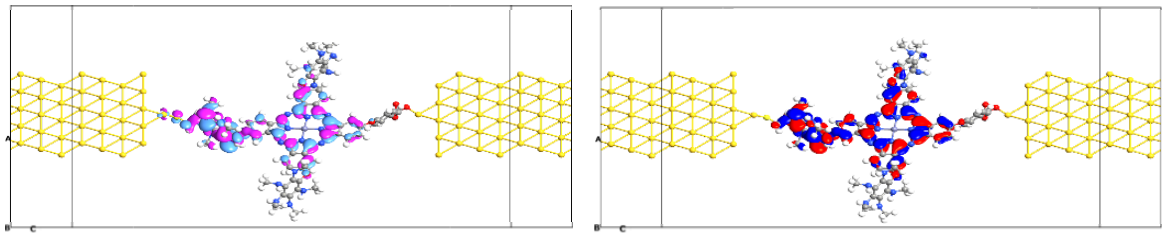


Transmission state = -0.36 eV



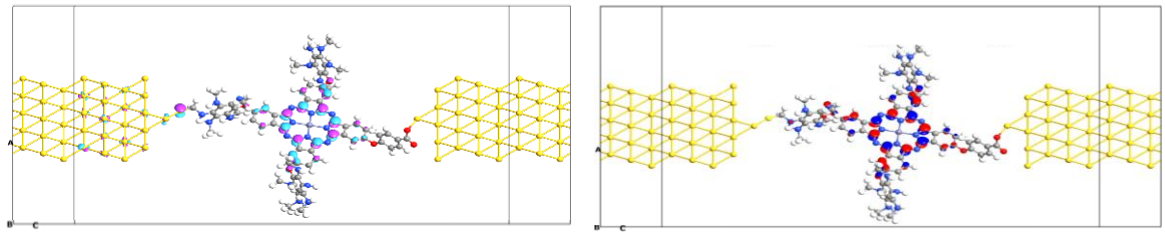
HOMO-1

ZnPc-3A



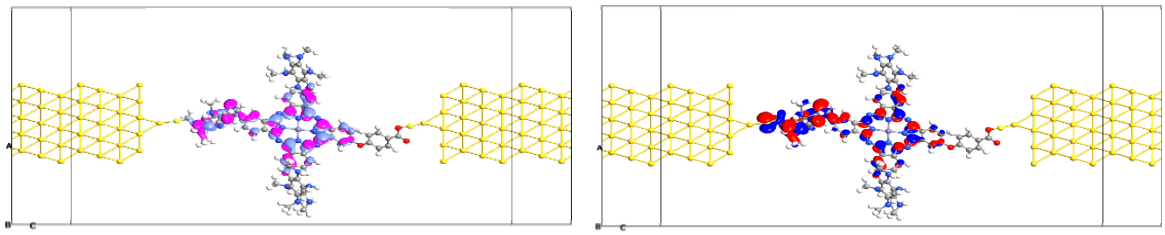
Transmission state = -0.800 eV HOMO-4

ZnPc-3B1



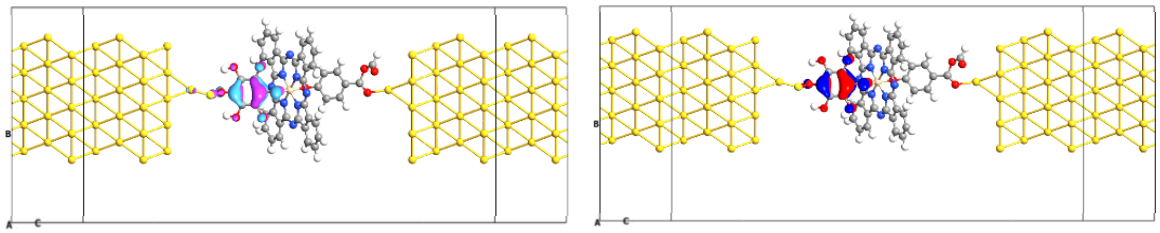
Transmission state = -0.688 eV HOMO-4

ZnPc-3B2



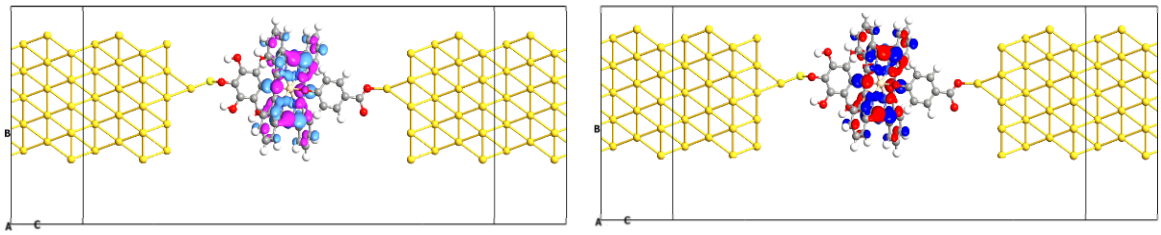
Transmission state = -0.760 eV HOMO-4

SiPc-1A



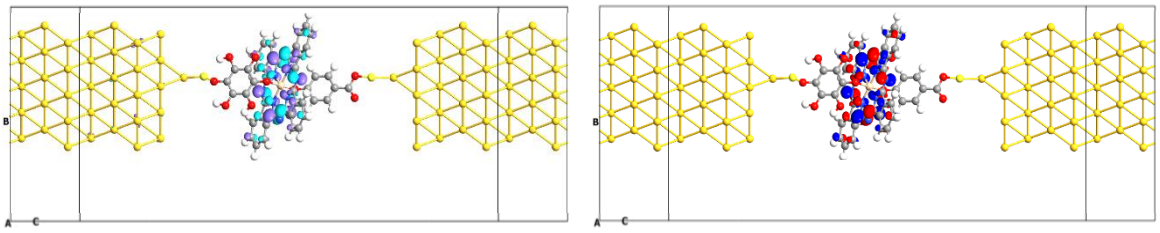
Transmission state = -0.752 eV HOMO-1

SiPc-1B1



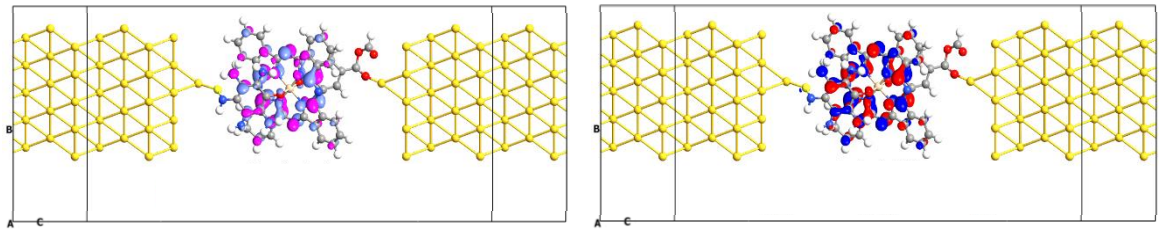
Transmission state = 0.584 eV LUMO

SiPc-1B2



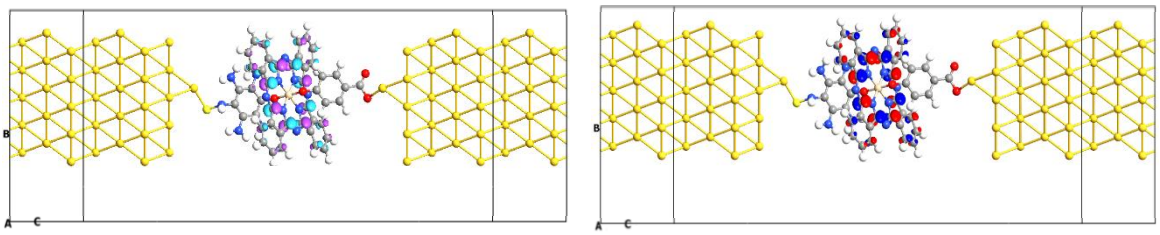
Transmission state = -0.616 eV | HOMO-1

SiPc-2A



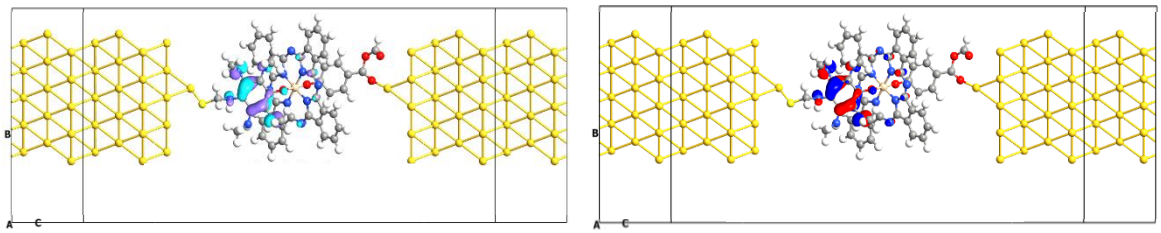
Transmission state = 0.344 eV | LUMO+2

SiPc-2B1



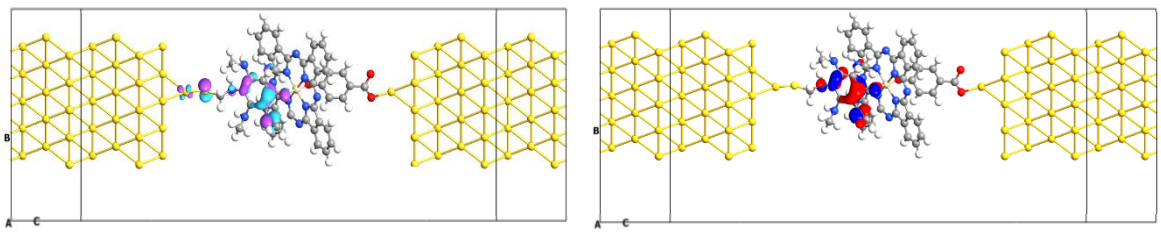
Transmission state = -1.136 eV | HOMO-3

SiPc-3A



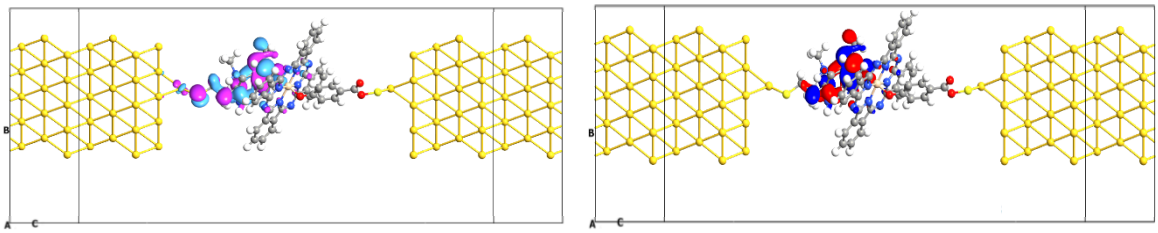
Transmission state = -0.264 eV | HOMO

SiPc-3B1



Transmission state = -0.520 eV | HOMO-2

SiPc-3B2



Transmission state = -0.496 eV | HOMO-2

Figure S4. Orbitals calculated under the influence of gold electrodes: **Left:** transmission orbital and **right:** molecular orbital.