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Supporting Information

for

Role of titanium and organic precursors in molecular layer deposition of “titanicone” hybrid materials

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Additional data on the geometry of the structures

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Table S1: Computed T–O distances between $TiCl_4$ and the anatase/rutile TiO_2 surface

Structure	Ti-O distance (Å)	Structure	Ti-O distance (Å)
A–$TiCl_3$	1.72	R–$TiCl_3$	1.74
A–$TiCl_2$	1.78, 1.78	R–$TiCl_2$	1.78, 1.81

Table S2: Computed Ti–O distances between EG and GL and the $TiCl_3$/$TiCl_2$-terminated anatase/ rutile TiO_2 surface and $TiCl_3$/$TiCl_2$ species with surface oxygens after the introduction of EG and GL

Structure	Ti–O (of EG, GL) distance (Å)	Ti–O (of surface) distance (Å)	Structure	Ti–O (of EG, GL) distance (Å)	Ti–O (of surface) distance (Å)
A–$TiCl_3$–EG	1.82	1.75	R–$TiCl_3$–EG	1.80	1.76
A–$TiCl_3$–GL	1.80	1.75	R–$TiCl_3$–GL	1.80	1.77
A–$TiCl_2$–EG	1.84	1.80, 1.81	R–$TiCl_2$–EG	1.82	1.82, 1.82
A–$TiCl_2$–GL	1.82	1.81, 1.81	R–$TiCl_2$–GL	1.82	1.83, 1.82

Table S3: Computed Ti–O distances between EG and GL in the upright and flat laying configuration and the $TiCl_3$-terminated anatase/rutile TiO_2 surface

Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)
A–$TiCl_3$–EG–up	1.80	R–$TiCl_3$–EG–up	1.81
A–$TiCl_3$–EG–flat	1.81	R–$TiCl_3$–EG–flat	1.84
A–$TiCl_3$–GL–up	1.80	R–$TiCl_3$–GL–up	1.82
A–$TiCl_3$–GL–flat	1.81	R–$TiCl_3$–GL–flat	1.88

Table S4: Computed Ti–O distances between $Ti(DMA)_4$ and the anatase/rutile TiO_2 and Al_2O_3 surfaces

Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)
A–$(DMA)_3$	1.91	R–$(DMA)_3$	1.79	Al_2O_3–$(DMA)_3$	1.73
A–$(DMA)_2$	1.91, 1.91	R–$(DMA)_2$	1.82, 1.85	Al_2O_3–$(DMA)_2$	1.79, 1.80
A–DMA	1.91, 1.98. 2.03	R–DMA	1.86, 1.86, 2.27	Al_2O_3–DMA	1.83, 1.83, 1.8

Table S5: Computed Ti–O distances between EG and GL with the TiDMA terminated anatase/rutile TiO_2 and Al_2O_3 surfaces

Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)
A–DMA–EG	1.80	R–DMA–EG	1.80	Al_2O_3–DMA–EG	1.86
A–DMA–GL	1.79	R–DMA–EG	1.80	Al_2O_3–DMA–EG	1.87

Table S6: Computed Ti–O distances between TDMAT and the anatase/rutile TiO_2 and Al_2O_3 surfaces after the introduction of EG and GL

Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)
A–DMA–EG	1.90, 1.98, 2.0	R–DMA–EG	1.86, 1.87, 2.23	Al_2O_3–DMA –EG	1.84, 1.85, 1.85
A–DMA–GL	1.91, 1.98, 2.0	R–DMA–EG	1.86, 1.87, 2.21	Al_2O_3– DMA–EG	1.83, 1.85, 1.85

Table S7: Computed Ti–O distances between EG and GL in the upright and flat laying configuration and the TiDMA-terminated anatase/rutile TiO_2 and Al_2O_3 surfaces

Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)	Structure	Ti–O distance (Å)
A–DMA–EG–up	1.80	R–DMA–EG–up	1.79	Al_2O_3–DMA –EG–up	1.87
A–DMA–EG–flat	1.88	R–DMA–EG–flat	1.85	Al_2O_3–DMA –EG–flat	2.08
A–DMA–GL–up	1.79	R–DMA–GL–up	1.79	Al_2O_3–DMA –GL–up	1.86
A–DMA–GL lat	1.86	R–DMA–GL–flat	1.84	Al_2O_3–DMA –GL–flat	2.11