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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

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 $\text{TiCl}_3/\text{TiCl}_2$ -terminated anatase/rutile TiO_2 surface and $\text{TiCl}_3/\text{TiCl}_2$ 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 TiCl₃-terminated anatase/rutile TiO₂ 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 TiO₂ and Al₂O₃ 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 ₂ O ₃ –(DMA) ₃	1.73
A–(DMA) ₂	1.91, 1.91	R–(DMA) ₂	1.82, 1.85	Al ₂ O ₃ –(DMA) ₂	1.79, 1.80
A–DMA	1.91, 1.98, 2.03	R–DMA	1.86, 1.86, 2.27	Al ₂ O ₃ –DMA	1.83, 1.83, 1.8

Table S5: Computed Ti–O distances between EG and GL with the TiDMA-terminated anatase/rutile TiO₂ and Al₂O₃ 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 ₂ O ₃ –DMA–EG	1.86
A–DMA–GL	1.79	R–DMA–EG	1.80	Al ₂ O ₃ –DMA–EG	1.87

Table S6: Computed Ti–O distances between TDMAT and the anatase/rutile TiO₂ and Al₂O₃ 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 ₂ O 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 ₂ O 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 TiO₂ and Al₂O₃ 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 ₂ O ₃ –DMA –EG–up	1.87
A–DMA–EG–flat	1.88	R–DMA–EG–flat	1.85	Al ₂ O ₃ –DMA –EG–flat	2.08
A–DMA–GL–up	1.79	R–DMA–GL–up	1.79	Al ₂ O ₃ –DMA –GL–up	1.86
A–DMA–GL lat	1.86	R–DMA–GL–flat	1.84	Al ₂ O ₃ –DMA –GL–flat	2.11